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FILE COVERS 1907 - 28 Sep 2007  VOL 147 ISS 15
FILE LAST UPDATED: 27 Sep 2007  (20070927/ED)

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  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

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L93           3 L55 OR L56

=> d ibib abs hitind hitstr L93 1-3

L93  ANSWER 1 OF 3  ZCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2005:216793  ZCAPLUS  Full-text
DOCUMENT NUMBER:          142:278860
TITLE:                    A method of isolating a thiol
INVENTOR(S):              Steenkamp, Daniel Jacobus
PATENT ASSIGNEE(S):       University of Cape Town, S. Afr.
SOURCE:                   PCT Int. Appl., 26 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
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     WO 2005021493         A2    20050310    WO 2004-IB2774           20040827
     WO 2005021493         A3    20050414
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
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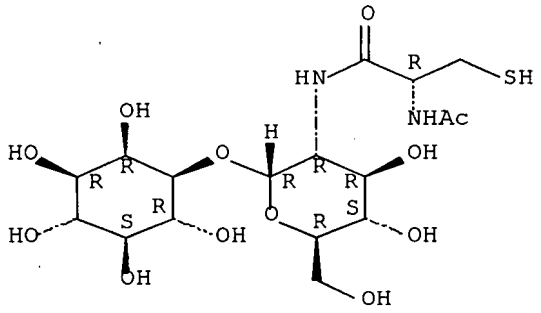
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

PRIORITY APPLN. INFO.: ZA 2003-6684 A 20030827
OTHER SOURCE(S): MARPAT 142:278860

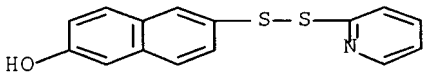
AB The invention relates to a method of isolating a ***thiol*** R'SH from a ***thiol*** containing mixture The method includes the steps of forming a mixed ***disulfide*** R'SSR of the ***thiol*** R'SH, ***purifying*** the mixed ***disulfide*** R'SSR and reducing the ***purified*** mixed ***disulfide*** R'SSR. The ***thiol*** R'SH is thereafter isolated. The invention extends to a ***disulfide*** of the formula R'SSR.

IC ICM C07C381-00
CC 16-1 (Fermentation and Bioindustrial Chemistry)
ST ***thiol purifn*** fermn ***disulfide*** deriv
IT Fermentation
Mycobacterium smegmatis
(***isolating*** a ***thiol*** from fermentation)
IT ***Thiols, preparation***
RL: BMF (Bioindustrial manufacture); ***PUR (Purification or recovery)***; RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(***isolating*** a ***thiol*** from fermentation)
IT ***192126-76-4P, Mycothiol***
RL: BMF (Bioindustrial manufacture); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(***isolating*** a ***thiol*** from fermentation)
IT 3483-12-3, Dithiothreitol
RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(***isolating*** a ***thiol*** from fermentation)
IT ***709044-44-0P 847493-45-2P***, 2-S-***Mycothiolyl***
-6-hydroxynaphthalene ***disulfide***
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(***isolating*** a ***thiol*** from fermentation)
IT 70-18-8, Glutathione, reactions ***6088-50-2 105988-28-1***,
2-Pyridinesulfenothioic acid ***847493-44-1***
RL: RCT (Reactant); RACT (Reactant or reagent)
(***isolating*** a ***thiol*** from fermentation)
IT ***847493-46-3P***, 2-S-Glutathionyl-6-hydroxynaphthalene
disulfide
RL: SPN (Synthetic preparation); PREP (Preparation)
(***isolating*** a ***thiol*** from fermentation)
IT ***192126-76-4P, Mycothiol***
RL: BMF (Bioindustrial manufacture); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(***isolating*** a ***thiol*** from fermentation)
RN 192126-76-4 ZCAPLUS
CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-mercapto-1-oxopropyl]amino]-2-deoxy-α-D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT ***709044-44-0P 847493-45-2P***, 2-S-***Mycothiolyl***
-6-hydroxynaphthalene ***disulfide***
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(***isolating*** a ***thiol*** from fermentation)
RN 709044-44-0 ZCAPLUS
CN 2-Naphthalenol, 6-(2-pyridinyldithio)- (9CI) (CA INDEX NAME)



RN 847493-45-2 ZCAPLUS
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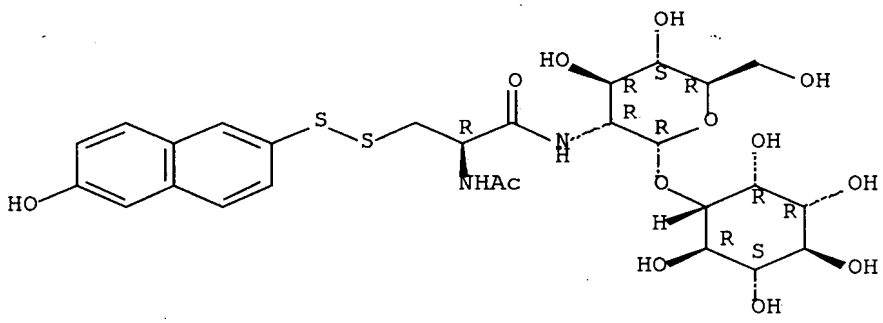
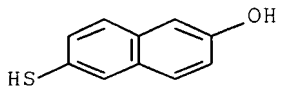
Absolute stereochemistry.



IT ***6088-50-2 105988-28-1***, 2-Pyridinesulfenothioic acid
847493-44-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(***isolating*** a ***thiol*** from fermentation)
RN 6088-50-2 ZCAPLUS
CN 2-Naphthalenol, 6-mercapto- (9CI) (CA INDEX NAME)



RN 105988-28-1 ZCAPLUS
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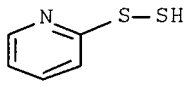

RN 847493-44-1 ZCAPLUS
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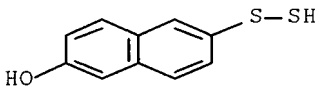
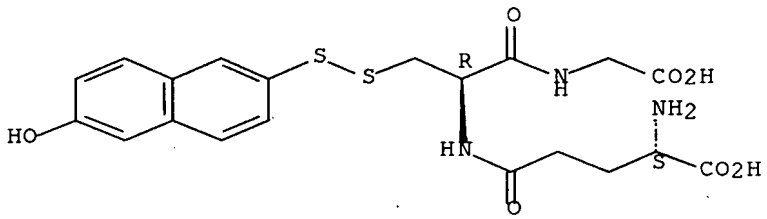


IT ***847493-46-3P***, 2-S-Glutathionyl-6-hydroxynaphthalene ***disulfide***
RL: SPN (Synthetic preparation); PREP (Preparation)
(***isolating*** a ***thiol*** from fermentation)
RN 847493-46-3 ZCAPLUS
CN Glycine, L-γ-glutamyl-3-[(6-hydroxy-2-naphthalenyl)dithio]-L-alanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L93 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:30260 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:50006
TITLE: Preparation and utilization of a reagent for the ***isolation*** and ***purification*** of low-molecular-mass ***thiols***
AUTHOR(S): ***Steenkamp, Daniel J.***; Vogt, Ryan N.

CORPORATE SOURCE: Faculty of Health Sciences, Division of Chemical Pathology, University of Cape Town, Cape Town, 7935, S. Afr.

SOURCE: Analytical Biochemistry (2004), 325(1), 21-27
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Elsevier Science
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Problems inherent in the isolation of ***thiols*** from natural sources, such as oxidation, undesirable addition reactions, and low concentration of ***thiol*** species in cell-free exts., can be circumvented by reversible derivatization to a less labile form which can be concentrated selectively. These objectives are realized by converting ***thiols*** to ***heterodisulfides*** in which the ***thiol*** partner is an apolar ***thiol*** with strong affinity for hydrophobic stationary phases. When reacted with 2-S-(2'-thiopyridyl)-6- ***hydroxynaphthyldisulfide*** at pH<5, where most ***thiol*** species are relatively stable to atmospheric oxidation, mixed ***disulfides*** with 2-mercapto-6-hydroxynaphthalene as the apolar partner are obtained in good yield and can be concentrated onto a hydrophobic stationary phase. Such ***heterodisulfides*** exhibit excellent chromatog. properties when separated on reversed-phase media and the derivatization reaction can, therefore, be conveniently monitored. Following their isolation as the ***heterodisulfides*** the ***thiol*** species of interest are recovered by reduction and facile separation from the apolar 2-mercapto-6-hydroxynaphthalene partner.

CC 9-15 (Biochemical Methods)
Section cross-reference(s): 80

ST reagent ***thiol*** thiopyridyl ***hydroxynaphthyldisulfide*** ***mycothiol*** glutathione glutathionylspermidine redn oxidn

IT Oxidation
Reduction
(preparation and utilization of reagent for ***isolation*** and ***purification*** of low-mol.-mass ***thiols*** from biol. system)

IT 70-18-8, Glutathione, analysis 3483-12-3, DTT 33932-35-3, Glutathionylspermidine ***192126-76-4, Mycothiol***
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(preparation and utilization of reagent for ***isolation*** and ***purification*** of low-mol.-mass ***thiols*** from biol. system)

IT ***709044-44-0***
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(preparation and utilization of reagent for ***isolation*** and ***purification*** of low-mol.-mass ***thiols*** from biol. system)

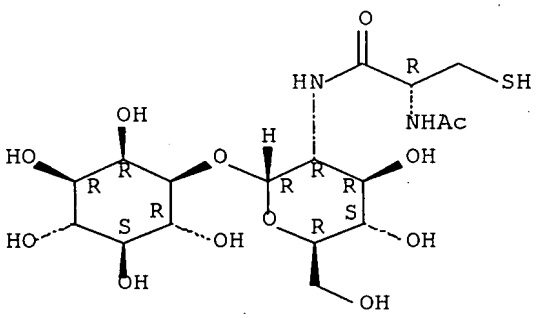
IT ***6088-50-2***
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation and utilization of reagent for ***isolation*** and ***purification*** of low-mol.-mass ***thiols*** from biol. system)

IT ***192126-76-4, Mycothiol***
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(preparation and utilization of reagent for ***isolation*** and ***purification*** of low-mol.-mass ***thiols*** from biol. system)

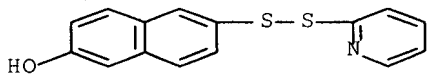
RN 192126-76-4 ZCAPLUS

CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-mercapto-1-oxopropyl]amino]-2-deoxy-α-D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT ***709044-44-0***
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(preparation and utilization of reagent for ***isolation*** and ***purification*** of low-mol.-mass ***thiols*** from biol. system)
RN 709044-44-0 ZCAPLUS
CN 2-Naphthalenol, 6-(2-pyridinyldithio)- (9CI) (CA INDEX NAME)



IT ***6088-50-2***
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation and utilization of reagent for ***isolation*** and ***purification*** of low-mol.-mass ***thiols*** from biol. system)
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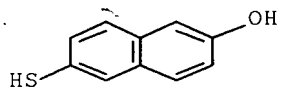

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:529567 ZCAPLUS Full-text
DOCUMENT NUMBER: 121:129567
TITLE: Identification of a major low-molecular-mass ***thiol*** of the trypanosomatid Crithidia fasciculata as ***ovothiol*** A. Facile isolation and structural analysis of the bimane derivative
AUTHOR(S): ***Steenkamp, Daniel J.***; Spies, Hendrik S. C.
CORPORATE SOURCE: Med. Sch., Univ. Cape Town, S. Afr.
SOURCE: European Journal of Biochemistry (1994), 223(1), 43-50
CODEN: EJBCAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal
LANGUAGE: English

AB An unidentified low-mol.-mass ***thiol***, U23, previously detected as the 7-diethylamino-3-(4'-maleimidylphenyl)-4-methylcoumarin derivative in exts. of the trypanosome Crithidia fasciculata, was ***purified*** as the bimane derivative Resonances attributable to U23 were discerned from those of the bimane label by comparison of the 1H- and 13C-NMR spectra of monobromobimane and U23-bimane. The complete 1H- and 13C-NMR spectra of U23-bimane were assigned by 1H-1H correlation spectroscopy, 1H-13C correlation spectroscopy and 13C multiplicity detns. The results indicated identity of U23 with 1-N-methyl-4-mercaptohistidine (***ovothiol*** A), previously isolated from marine sources. This assignment was confirmed by NOE difference expts., fast-atom-bombardment mass spectrometry of U23-bimane and UV/visible spectrophotometry of U23, which was isolated as the ***disulfide***. The isolation of ***ovothiol*** A from a parasitic protozoan suggest that the 4-mercaptohistidines may have a wider distribution and function as antioxidant ***thiols*** than was hitherto realized.

CC 10-1 (Microbial, Algal, and Fungal Biochemistry)
Section cross-reference(s): 6

ST ***ovothiol*** A Crithidia

IT Crithidia fasciculata
(***ovothiol*** A of, identification and characterization of)

IT 108418-13-9, ***Ovothiol*** A
RL: BIOL (Biological study)
(of Crithidia fasciculata, identification and characterization of)

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Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available.  If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

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DICTIONARY FILE UPDATES:  27 SEP 2007  HIGHEST RN 948530-59-4

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FILE COVERS 1907 - 28 Sep 2007  VOL 147 ISS 15
FILE LAST UPDATED: 27 Sep 2007  (20070927/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

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L17          147 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  DI SULFID?/BI
L18         1626 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  BISULFID?/BI OR BI SULFID?/BI

L19           11 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L15 AND (L16 OR L17 OR L18)
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L9             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  105988-28-1
L10            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-44-1
L11            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-46-3
L24       120255 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?DISULFID?/BI
L25       167140 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?THIOL?/BI
L26        20268 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L24 AND L25
L31           14 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L3 OR L5 OR L6 OR (L8 OR L9
                 OR L10 OR L11)) AND L26
L35            2 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L31 AND ?ISOLAT?/OBI


=> d stat que L36
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L5             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  709044-44-0
L6             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-45-2
L8             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  6088-50-2
L9             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  105988-28-1
L10            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-44-1
L11            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-46-3
L24       120255 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?DISULFID?/BI
L25       167140 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?THIOL?/BI
L26        20268 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L24 AND L25
L31           14 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L3 OR L5 OR L6 OR (L8 OR L9
                 OR L10 OR L11)) AND L26
L36            1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L31 AND TOTAL/TI


=> d stat que L37
L3             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  192126-76-4
L5             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  709044-44-0
L6             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-45-2
L8             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  6088-50-2
L9             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  105988-28-1
L10            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-44-1
L11            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-46-3
L24       120255 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?DISULFID?/BI
L25       167140 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?THIOL?/BI
L26        20268 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L24 AND L25
L31           14 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L3 OR L5 OR L6 OR (L8 OR L9
                 OR L10 OR L11)) AND L26
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L37             1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L31 AND REDUCTION?/TI


=> d stat que L23
L14        264757 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PUR/RL
L20          3625 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  DISULFIDES/CT
L21             7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L20 (L) L14
L22        167140 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?THIOL?/BI
L23             1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L21 AND L22


=> d stat que L58
L14        264757 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PUR/RL
L20          3625 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  DISULFIDES/CT
L21             7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L20 (L) L14
L39        166847 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?MERCAPT?/BI
L58             3 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L39 AND L21


=> d stat que L62
L5              1 SEA FILE=REGISTRY ABB=ON  PLU=ON  709044-44-0
L6              1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-45-2
L11             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-46-3
L59             2 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L5
L60             1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L6
L61             1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L11
L62             2 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L59 OR L60 OR L61)


=> d stat que L69
L8              1 SEA FILE=REGISTRY ABB=ON  PLU=ON  6088-50-2
L10             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  847493-44-1
L63             9 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L8
L64             1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L10
L65             9 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L63 OR L64)
L68         15061 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  MERCAPTO GROUP/CT
L69             1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L65 AND L68


=> d stat que L71
L3              1 SEA FILE=REGISTRY ABB=ON  PLU=ON  192126-76-4
L71             2 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L3/PUR


=> s (L33 or L35 or L36 or L37 or L23 or L58 or L62 or L69 or L71) not L55-L56
L94            13 (L33 OR L35 OR L36 OR L37 OR L23 OR L58 OR L62 OR L69 OR L71)
                  NOT (L55 OR L56)

=> file casreact
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FILE CONTENT:1840 - 22 Sep 2007 VOL 147 ISS 14
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=> d stat que L89
L86         1384 SEA FILE=CASREACT ABB=ON  PLU=ON  THIOL/FG.RCT (L) DISULFIDE/FG
                 .PRO
L87          505 SEA FILE=CASREACT ABB=ON  PLU=ON  DISULFIDE/FG.RCT (L)
                 THIOL/FG.PRO
L89           12 SEA FILE=CASREACT ABB=ON  PLU=ON  L86 (L) L87


=> dup rem L94 L89
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PROCESSING COMPLETED FOR L94
PROCESSING COMPLETED FOR L89
L95           25 DUP REM L94 L89 (0 DUPLICATES REMOVED)
                 ANSWERS '1-13' FROM FILE ZCAPLUS
                 ANSWERS '14-25' FROM FILE CASREACT

=> d ibib abs hitind hitstr L95 1-13; d ibib abs hit L95 14-25

L95  ANSWER 1 OF 25  ZCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2004:553613  ZCAPLUS  Full-text
DOCUMENT NUMBER:          141:239461
TITLE:                    Isolation and structure assignments of rostratins A-D,
                          cytotoxic disulfides produced by the marine-derived
                          fungus Exserohilum rostratum
AUTHOR(S):                Tan, Ren Xiang; Jensen, Paul R.; Williams, Philip G.;
                          Fenical, William
CORPORATE SOURCE:         Center for Marine Biotechnology and Biomedicine,
                          Scripps Institution of Oceanography, University of
                          California, La Jolla, CA, 92093-0204, USA
SOURCE:                   Journal of Natural Products (2004), 67(8), 1374-1382
                          CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
GI
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four new cytotoxic disulfides, rostratins A-D (I-IV), were isolated from the whole broth of the marine-derived fungus E. rostratum (Drechsler), a fungal strain found associated with a marine cyanobacterial mat. The structures of these cyclic dipeptides were established through chemical degradation and a variety of 2-dimensional NMR techniques. The absolute configurations of the rostratins were determined by the modified Mosher method. In the case of the polyhydroxylated compound I and the ***mercaptol*** IV, regioselective acylation was achieved by modulating the reaction temperature while monitoring the progress of the reaction by 1H NMR. I, II, III, and IV showed in vitro cytotoxicity against human colon carcinoma (HCT-116) with IC50 values of 8.5, 1.9, 0.76, and 16.5 μg/mL, resp.

CC 10-1 (Microbial, Algal, and Fungal Biochemistry)

IT ***Disulfides***
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); ***PUR (Purification or recovery)***; BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(rostratins A-D are cytotoxic disulfides produced by the marine-derived fungus Exserohilum rostratum)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 2 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:42415 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:253784
TITLE: First ***Total*** Synthesis of ***Mycothiol*** and ***Mycothiol Disulfide***
AUTHOR(S): Lee, Sungwon; Rosazza, John P. N.
CORPORATE SOURCE: Division of Medicinal and Natural Products Chemistry, College of Pharmacy, and Center for Biocatalysis and Bioprocessing, University of Iowa, Iowa City, IA, 52242, USA
SOURCE: Organic Letters (2004), 6(3), 365-368
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:253784

AB The first total synthesis of ***mycothiol*** and ***mycothiol disulfide*** was achieved by linking D-2,3,4,5,6-penta-O-acetyl-myo- inositol, O-(3,4,6-tri-O-acetyl-2-azido-2-deoxy-α,β-D- glucopyranosyl)trichloroacetimidate, and N,S-diacetyl-L-cysteine and deprotecting peracetylated ***mycothiol***. The first full spectral characterization is reported for underivatized ***mycothiol***. The structure of ***mycothiol*** was confirmed by spectral anal. of the known bimane derivative

CC 33-7 (Carbohydrates)
Section cross-reference(s): 34

ST inositol azidodeoxyglucopyranose acetylcysteine conjugation ***mycothiol*** synthesis; ***mycothiol*** sulfide bimane total synthesis

IT Cyclitols
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(first total synthesis of ***mycothiol*** and ***mycothiol disulfide***)

IT Molecular structure
(of ***mycothiol***)

IT ***192126-76-4P***
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)
(first total synthesis of ***mycothiol*** and ***mycothiol disulfide***)

IT 52-89-1, L-Cysteine hydrochloride 87-89-8, myo-Inositol 1122-84-5, 1-Ethoxycyclohexene 2873-29-2, Tri-O-acetyl-D-glucal 39637-74-6, (-)-Camphanic chloride 71418-44-5, Monobromobimane 145626-87-5, Bis(2-mercaptoethyl)sulfone
RL: RCT (Reactant); RACT (Reactant or reagent)
(first total synthesis of ***mycothiol*** and ***mycothiol disulfide***)

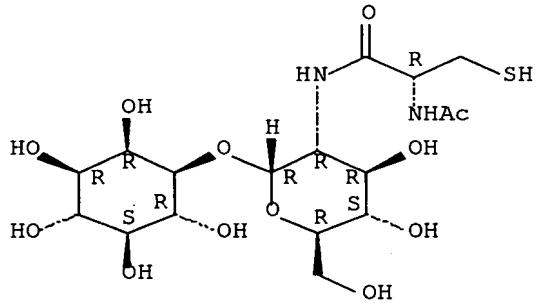
IT 18725-37-6P 35519-39-2P 38183-33-4P 104873-71-4P 111901-82-7P 111901-83-8P 120202-94-0P 145840-43-3P 187726-63-2P 668481-13-8P 668481-14-9P 668481-15-0P 668481-16-1P 669091-43-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(first total synthesis of ***mycothiol*** and ***mycothiol disulfide***)

IT 158761-05-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(first total synthesis of ***mycothiol*** and ***mycothiol disulfide***)

IT ***192126-76-4P***
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(first total synthesis of ***mycothiol*** and ***mycothiol disulfide***)

RN 192126-76-4 ZCAPLUS
CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-mercapto-1-oxopropyl]amino]-2-deoxy-α-D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 3 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:706948 ZCAPLUS Full-text
DOCUMENT NUMBER: 137:372244
TITLE: Mercaptans from Gas Condensates and Crude Oils
AUTHOR(S): Sharipov, A. Kh.
CORPORATE SOURCE: Institute of Petrochemistry and Catalysis, Academy of Sciences of the Republic of Bashkortostan and Urals Science Center, Russia
SOURCE: Chemistry and Technology of Fuels and Oils (Translation of Khimiya i Tekhnologiyà Topliv i Masel)

(2002), 38(4), 280-285
CODEN: CTFOAK; ISSN: 0009-3092
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review on the occurrence of mercaptans in natural gas and petroleum and technologies for removal. Industrial separation schemes are described, and promising areas of application of mercaptans from gas condensate and kerosene distillates of medium-sulfur crude oils are noted. The fields of mercaptan-containing gas condensates and crude oils in regions confined to the Caspian Sea basin opened up with the development of deep drilling technol. For example, the Markovo field in East siberia has a high mercaptan content, 0.5-0.7%, the majority of the sulfur present, and has an absence of elemental sulfur, sulfide, and ***disulfide*** species. The Caspian Sea fields are also high in mercaptan sulfur and low in inorg. forms. Production of heavy carbonaceous crudes containing up to 50-80 ppm Me- and ethylmercaptans is increasing at high rates in the region between the Volga and the Urals, with even higher Et mercaptan concentration in the gas condensates. The mercaptans are extracted with alkali forming sodium salts, sent to another tower where they are thermally decomposed back into alkali and mercaptans. Currently in Russia, much of the mercaptans are wasted. Various strategies for com. products made from these mercaptans are presented. For example, methylmercaptan can be used to produce synthetic methionine by reacting with acrolein to form an aldehyde intermediate, reducing toxicity and odor of outgoing product shipments, but currently in Russia this material is mostly burned at the natural gas processing plants. Another example describes catalytic conversion to alkyl ***disulfides***.

CC 51-0 (Fossil Fuels, Derivatives, and Related Products)

IT ***Disulfides***
RL: IMF (Industrial manufacture); PREP (Preparation)
(alkyl derivs.; recovery and uses of mercaptans from gas condensates and crude oils)

IT ***Thiols, preparation***
RL: GOC (Geological or astronomical occurrence); ***PUR (Purification or recovery)***; REM (Removal or disposal); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(recovery and uses of mercaptans from gas condensates and crude oils)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 4 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:770996 ZCAPLUS Full-text
DOCUMENT NUMBER: 135:305979
TITLE: Process for removing sulfur compounds from hydrocarbon streams
INVENTOR(S): Pittman, Rusty; Arena, Blaise J.; Janssen, Albert J.
PATENT ASSIGNEE(S): UOP LLC, USA
SOURCE: U.S., 6 pp., Cont.-in-part of U.S. Ser. No. 61,661, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6306288	B1	20011023	US 1999-426818	19991022
EG 22909	A	20031030	EG 2001-669	20010620
JP 2003226881	A	20030815	JP 2001-189890	20010622

JP 2003027068	A	20030129	JP 2001-191421	20010625
EP 1270704	A1	20030102	EP 2001-115343	20010626
EP 1270704	B1	20060927		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
AT 340837	T	20061015	AT 2001-115343	20010626
PRIORITY APPLN. INFO.:			US 1998-61661	B2 19980417
			US 1999-426818	A 19991022
			EP 2001-115343	A 20010626

AB A process for removing H2S and ***mercaptans*** from a hydrocarbon stream is disclosed. A hydrocarbon stream such as a LPG stream is contacted with a weakly basic stream, e.g., a Na bicarbonate stream to extract the H2S and ***mercaptans*** from the hydrocarbon stream into the basic stream. The basic stream is now treated in a reactor containing a sulfide-oxidizing microorganism to convert the H2S to S and the ***mercaptans*** to disulfides. Finally, the S and disulfides are separated from the basic aqueous stream which can be recycled and used to treat a fresh hydrocarbon stream. The treated hydrocarbon stream is purified to the point that it passes the Cu strip test, while the purified basic stream contains <0.08 g S/L.

IC ICM C10G019-08
ICS C10G019-00; C10G032-00

INCL 208235000

CC 51-4 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 49

ST sulfur compd removal hydrocarbon; hydrogen sulfide removal LPG; ***mercaptan*** removal LPG

IT ***Disulfides***
RL: ***PUR (Purification or recovery)***; PREP (Preparation)
(recovery in removing of sulfur compds. from hydrocarbon streams)

IT ***Thiols*** (organic), processes
RL: REM (Removal or disposal); PROC (Process)
(removing of sulfur compds. from hydrocarbon streams)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 5 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:381217 ZCAPLUS Full-text
DOCUMENT NUMBER: 135:166575
TITLE: Unexpected Catalyzed C:C Bond Cleavage by Molecular Oxygen Promoted by a Thiyl Radical
AUTHOR(S): Baucherel, Xavier; Uziel, Jacques; Juge, Sylvain
CORPORATE SOURCE: Unite Mixte Universite de Cergy Pontoise-ESCOM FRE CNRS 2126 Synthese Organique Selective et Chimie Organometallique, Cergy Pontoise, 95031, Fr.
SOURCE: Journal of Organic Chemistry (2001), 66(13), 4504-4510
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:166575

AB Olefin oxidation with mol. oxygen, promoted by a transition metal catalyst and a thiophenol, involved C:C bond cleavage into the corresponding carbonyl derivs. This new reaction proceeds under one atmospheric of oxygen, at room temperature, in the presence of an excess of thiophenol and a catalyst such as MnL2 3a or VClL2 3c. It was applied to aromatic and aliphatic olefins, as well as to functionalized or unfunctionalized acyclic compds., providing the corresponding ketones and aldehydes in up to 98% yield. The synthetic interest of this catalytic oxidation was illustrated by a one-step preparation of the fragrance (-)-4-acetyl-1-methylcyclohexene 7e in 73% isolated yield. The C:C bond cleavage probably results from a catalyzed decomposition of the

β-hydroperoxysulfide intermediate that is formed by the radical addition of thiophenol to the olefin in the presence of oxygen. Although an excess of the thiophenol was used, it was transformed into the ***disulfide*** which could then be reduced without purification in 83% overall yield, thereby allowing for recycling. In addition, the C:C bond cleavage under oxygen could be promoted by catalytic quantities of the thiyl radical, generated by photolysis of the ***disulfide***; thus, in the presence of 0.1 equiv of bis(4-chlorophenyl) ***disulfide*** 4b and 5% of the manganese complex 3a, trans-methylstilbene gave, under radiation, benzaldehyde and acetophenone in up to 95% yield. This new reaction offers an alternative to the classical C:C bond cleavage procedures, and further developments in the fields of bioinorg. and environmental chemical are likely.

CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 30, 62

IT Aromatic hydrocarbons, reactions
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(aryl alkenes; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

IT ***Thiols (organic), reactions***
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); ***PUR (Purification or recovery)***; RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(aryl; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT Alkenes, reactions
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(aryl; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT ***Disulfides***
RL: CAT (Catalyst use); FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent); USES (Uses)
(formation and reduction under thermal conditions and catalytic activity under photolytic conditions)

IT Catalysts
Regiochemistry
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT Transition metal complexes
RL: CAT (Catalyst use); USES (Uses)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT Alkenes, reactions
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT Aldehydes, preparation
Ketones, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT Bond cleavage
(oxidative; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

IT Photolysis
(photoinduced C:C bond cleavage; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

IT Phenols, reactions
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(thiolphenols; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

IT 151930-49-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(catalytic ligand; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

IT 90-02-8, Salicylaldehyde, reactions 5619-04-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

IT 353736-48-8
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(not a bond cleavage intermediate; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

IT 1142-19-4, Bis(4-chlorophenyl) ***disulfide*** 7718-98-1, Vanadium trichloride 7773-01-5, Manganese dichloride
RL: CAT (Catalyst use); USES (Uses)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT 100-42-5, Styrene, reactions 103-30-0, trans-Stilbene 111-66-0, 1-Octene 140-10-3, trans-Cinnamic acid, reactions 447-53-0, 1,2-Dihydronaphthalene 530-48-3, 1,1-Diphenylethylene 623-91-6, Ethyl fumarate 645-49-8, cis-Stilbene 695-12-5, Vinylcyclohexane 833-81-8, trans-1,2-Diphenylpropene 4192-77-2, trans-Ethyl cinnamate 4407-36-7, trans-Cinnamyl alcohol 5989-54-8, (S)-(-)-Limonene 6094-02-6, 2-Methyl-1-hexene 7782-44-7, Oxygen, reactions 18172-67-3, (-)-β-Pinene
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC

(Process); RACT (Reactant or reagent)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT 98-86-2P, Acetophenone, preparation 100-52-7P, Benzaldehyde, preparation 111-71-7P, Heptanal 119-61-9P, Benzophenone, preparation 591-78-6P, 2-Hexanone 924-44-7P, Ethyl glyoxylate 2043-61-0P, Cyclohexanecarboxaldehyde 14807-28-4P 38651-65-9P, (+)-Nopinone 57072-59-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***
)

IT 106-54-7P, 4-Chlorothiophenol 7340-90-1P
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(reagent and recovery; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic ***disulfide***)

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 6 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:439719 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:204979
TITLE: Contamination of an anion-exchange membrane by glutathione
AUTHOR(S): Gotoh, Takeshi; Kikuchi, Ken-Ichi
CORPORATE SOURCE: Department of Materials-Process Engineering & Applied Chemistry for Environments, Faculty of Engineering and Resource Science, Akita University, Akita, 010-8502, Japan
SOURCE: Bioseparation (2000), 9(1), 37-41
CODEN: BISPE4; ISSN: 0923-179X
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Electrodialysis, which can sep. electrolytes under mild conditions by using ion-exchange membranes, is a strong candidate for separation of GSH from yeast exts., because GSH is unstable and easily oxidized forming a ***disulfide*** bond especially under alkali conditions. In this paper, sorption behavior of GSH on an anion-exchange membrane, in the pH 3-6 region that is expected to be the most preferable for its electrodialytic separation, was examined Sorption of GSH on a Selemion-AMV anion-exchange membrane was accelerated as the pH of the membrane-contact solution increased, and there was a good correlation between the sorbed amts. and the molar fraction of monovalent anionic species of GSH. However, the amts. of GSH desorbed from the membrane by a NaCl desorbing solution were much lower than the initial sorbed amts., and the difference between them was enlarged with increasing pH. The GSH which was lost could be recovered by the addition of DTT in the membrane-contact and desorbing solns. Similar results were also obtained with Cys. We thus concluded that an anion-exchange membrane would be contaminated by thiol compds., such as GSH and Cys, through oxidative binding of the thiol group with the membrane, the local OH- concentration in which was enhanced due to attraction by the pos. charged anion-exchange membrane.

CC 9-9 (Biochemical Methods)

Section cross-reference(s): 6, 34
IT ***Thiols (organic), biological studies***
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); ***PUR (Purification or recovery)***; BIOL (Biological study); PREP (Preparation); PROC (Process)
(contamination of anion-exchange membrane by glutathione)
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 7 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:341203 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:339677
TITLE: Process for preparing pure and stable solutions of organic thiols, sulfides and dithiocarbamates
INVENTOR(S): Svehla, Pavel; Zaludek, Borek; Rosicky, Lubor
PATENT ASSIGNEE(S): Lachema, A. S., Czech Rep.
SOURCE: Czech Rep., 4 pp.
CODEN: CZXXED
DOCUMENT TYPE: Patent
LANGUAGE: Czech
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CZ 283636	B6	19980513	CZ 1990-3560	19900718
PRIORITY APPLN. INFO.:			CS 1990-3560 A	19900718

AB Pure stable solns. of organic thiols, sulfides and dithiocarbaminates (e.g. sodium dimethyldithiocarbamate) are prepared from the corresponding crude organic compds. treatment with compds. (e.g., tetramethylthiuram ***disulfide*** and hydrazine sulfate) producing solid ***disulfides*** from the impurities at pH 10-12 followed by filtration of the solid ***disulfide*** impurity.
IC ICM C07C323-00
CC 45-1 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
IT ***Disulfides***
RL: BYP (Byproduct); REM (Removal or disposal); PREP (Preparation); PROC (Process)
(organic; removal of)
IT Thioethers
Thiols (organic), preparation
RL: ***PUR (Purification or recovery)***; PREP (Preparation)
(process for preparing pure and stable solns. of)
IT Filtration
(process for preparing pure and stable solns. of organic thiols and sulfides
and dithiocarbamates with solid ***disulfide*** removal by)
IT 87-90-1, Trichloroisocyanuric acid 137-26-8, Tetramethylthiuram ***disulfide*** 302-01-2, Hydrazine, reactions 7722-64-7, Potassium permanganate 7722-84-1, Hydrogen peroxide, reactions 7727-21-1, Potassium peroxydisulfate 7775-14-6, Sodium dithionite 7803-49-8, Hydroxylamine, reactions 10034-93-2, Hydrazine sulfate
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for preparing pure and stable solns. of organic thiols, sulfides and
dithiocarbamates)

L95 ANSWER 8 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:641496 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:328617

TITLE: General method to identify and enrich vicinal thiol proteins present in intact cells in the oxidized, ***disulfide*** state

AUTHOR(S): Gitler, Carlos; Zarmi, Batia; Kalef, Edna
CORPORATE SOURCE: Dep. Membrane Res. Biophysics, Weizmann Inst. Sci., Rehovot, 76100, Israel

SOURCE: Analytical Biochemistry (1997), 252(1), 48-55
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Some 5% of the soluble proteins of L1210 murine leukemia lymphoblasts contain surface vicinal thiols. Redox dithiol to intraprotein ***disulfide*** conversion could regulate the cellular function of these proteins. A general method is presented to identify and enrich vicinal thiol proteins existing in cells in their oxidized, ***disulfide*** state. The method is based on the in situ blockage by cell permeable N-ethylmaleimide (NEM) of readily accessible cellular protein sulfhydryls. Following removal of the excess NEM, ***disulfide***-containing proteins were identified by reduction with DTT and specific labeling with N-iodoacetyl-[125I]-3-iodotyrosine ([125I]IAIT). The vicinal thiol proteins formed could also be enriched, prior to labeling with [125I]IAIT, by their selective binding to Sepharose-aminohexanoyl-4-aminophenylarsine oxide. Exponentially growing L1210 lymphoblasts contain >20 proteins with thiols in the oxidized, ***disulfide*** state. The majority derive from vicinal thiol proteins. The fraction oxidized, in some proteins, represents almost the totality of the protein present in the cell. Exposure of lymphoblasts to diamide increases the number and concentration of proteins with intraprotein ***disulfides***. This method allows sensitive direct identification of vicinal thiol proteins that participate in redox regulation and those that are targets to oxidative stress conditions.

CC 9-16 (Biochemical Methods)
Section cross-reference(s): 4

IT Animal cell line
(L-1210; identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT Proteins, specific or class
RL: ANT (Analyte); PUR (Purification or recovery); ANST (Analytical study); PREP (Preparation)
(***disulfide***-containing; identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT Thiols (organic), biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(dithiols; identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT Lymphoblast
Oxidative stress, biological
(identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT ***Disulfides***
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT Proteins, specific or class
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(redox; identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT Proteins, specific or class
RL: ANT (Analyte); PUR (Purification or recovery); ANST (Analytical

study); PREP (Preparation)
(vicinal thiol-containing; identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT ***Thiols (organic), analysis***
RL: ANT (Analyte); ***PUR (Purification or recovery)***; ANST (Analytical study); PREP (Preparation)
(vicinal, proteins containing; identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT 128-53-0 150956-52-8
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT 1122-90-3D, 4-Aminophenylarsine oxide, linked to aminohexanoyl and Sepharose 4B 1319-82-0D, Aminohexanoic acid, linked to Sepharose 4B and 4-aminophenylarsine oxide 9012-36-6D, Sepharose 4B, linked to aminohexanoyl and 4-aminophenylarsine oxide
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

IT 3483-12-3, Dithiothreitol
RL: RCT (Reactant); RACT (Reactant or reagent)
(identification and enrichment of vicinal thiol proteins present in cells in oxidized ***disulfide*** state)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 9 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:58340 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:121805
TITLE: Separately removing ***mercaptans*** and hydrogen sulfide from gas streams with disulfide recovery
INVENTOR(S): Samuels, Alvin; Fox, Irwin
PATENT ASSIGNEE(S): USA
SOURCE: U.S., 5 pp. Cont.-in-part of U.S. 187,146, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

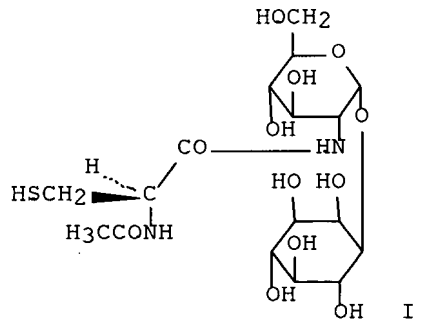
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5478541	A	19951226	US 1995-440114	19950512
PRIORITY APPLN. INFO.:			US 1995-440114	B2 19950512
			US 1994-187146	19940127

AB ***Mercaptans*** and hydrogen sulfide are removed sep. from a hydrocarbon gas stream by passing the gas through a bed which includes iron oxide (crystalline Fe3O4 and amorphous Fe2O3) which catalyzes the formation of disulfides and trisulfides from ***mercaptans*** and also reacts with at least part of the hydrogen sulfide to form acid-stable solids; causing the di- and trisulfides to exit the bed in the gas phase; and removing and recovering the di- and trisulfides by adsorption or condensation. Any remaining hydrogen sulfide may be scavenged from the gas stream by passage through a bed containing iron oxide similar to that used first above. If the gas stream contains substantial amts. of hydrocarbon aerosols, they should be filtered out in advance of the bed.

IC ICM C01B017-16
ICS C01B017-20
INCL 423220000
CC 51-5 (Fossil Fuels, Derivatives, and Related Products)

ST **mercaptan** removal hydrocarbon gas disulfide recovery
IT **Disulfides**
Trisulfides
RL: **PUR (Purification or recovery)**; REM (Removal or disposal); PREP (Preparation); PROC (Process)
(sep. removing **mercaptans** and hydrogen sulfide from gas streams with disulfide recovery)
IT 7440-44-0, Carbon, uses
RL: NUU (Other use, unclassified); USES (Uses)
(activated; sep. removing **mercaptans** and hydrogen sulfide from gas streams with disulfide recovery)
IT 1309-37-1, Iron oxide (fe2o3), uses
RL: NUU (Other use, unclassified); USES (Uses)
(amorphous; sep. removing **mercaptans** and hydrogen sulfide from gas streams with disulfide recovery)
IT 1317-61-9, Iron oxide (fe3o4), uses
RL: NUU (Other use, unclassified); USES (Uses)
(crystalline; sep. removing **mercaptans** and hydrogen sulfide from gas streams with disulfide recovery)
IT 110-81-6P, Di ethyl disulfide 624-92-0P, Di methyl disulfide 3600-24-6P, Di ethyl trisulfide 3658-80-8P, Di methyl trisulfide 20333-39-5P, Methyl ethyl disulfide 31499-71-5P, Methyl ethyl trisulfide
RL: PUR (Purification or recovery); REM (Removal or disposal); PREP (Preparation); PROC (Process)
(sep. removing **mercaptans** and hydrogen sulfide from gas streams with disulfide recovery)
IT 74-93-1, Methyl **mercaptan**, processes 75-08-1, Ethyl **mercaptan** 7783-06-4, Hydrogen sulfide, processes
RL: REM (Removal or disposal); PROC (Process)
(sep. removing **mercaptans** and hydrogen sulfide from gas streams with disulfide recovery)

L95 ANSWER 10 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:630956 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:140470
TITLE: The structure of U17 isolated from Streptomyces clavuligerus and its properties as an antioxidant thiol
AUTHOR(S): Newton, Gerald L.; Bewley, Carole A.; Dwyer, Tammy J.; Horn, Ronda; Aharonowitz, Yair; Cohen, Gerald; Davies, Julian; Faulkner, D. John; Fahey, Robert C.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA, 92093-0506, USA
SOURCE: European Journal of Biochemistry (1995), 230(2), 821-5
CODEN: EJBCAI; ISSN: 0014-2956
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The predominant low-mol.-mass thiol produced by streptomycetes is a cysteine derivative previously designated as U17. In this study the elucidation of the structure of the monobromobimane derivative of U17 (I) is reported, which establishes the structure of U17 as 2-(N- acetylcysteinyl)amido-2-deoxy-α-D-glucopyranosyl-myo-inositol. The presence of the N-acetylcysteine moiety was indicated by formation of N-acetylcysteine-monobromobimane during acid hydrolysis of I. Complete hydrolysis of I released 1 mol glucosamine/mol cysteine as determined by carbohydrate and amino acid anal. High-resolution mass spectral anal. gave a precise mass consistent with the mol. formula C27H40N4O14S. Anal. of 13C-NMR, 1-dimensional 1H-NMR and 2-dimensional NMR expts. identified the remaining C6H12O6 moiety as myo-inositol, confirmed the presence of N-acetyl-cysteine and glucosamine, and established the connectivity of the components. Two chemical properties of this novel thiol, which is equated to mycothiol from Mycobacterium bovis, make it suitable as an intracellular storage form of cysteine and as an antioxidant thiol. First, it undergoes heavy-metal-ion catalyzed autoxidn. at a rate dramatically lower than that for cysteine and markedly lower than that for glutathione or N-acetylcysteine. Secondly, the α-(1→1) glycosidic link between glucosamine and myo-inositol is resistant to acid hydrolysis, hydrolyzing at a rate comparable to that of the 2 amide bonds in the mol.

CC 10-1 (Microbial, Algal, and Fungal Biochemistry)

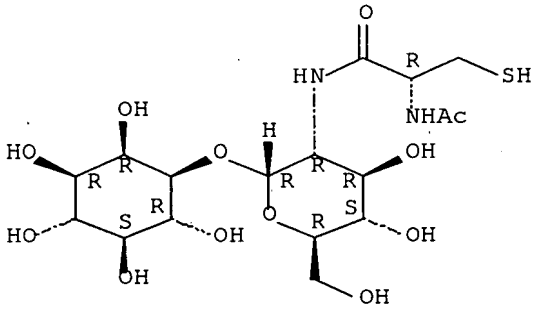
IT 158761-05-8P ***192126-76-4P***, Mycothiol
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); ***PUR (Purification or recovery)***; BIOL (Biological study); PREP (Preparation); PROC (Process)
(structure of U17 (mycothiol) isolated from Streptomyces clavuligerus and its properties as an antioxidant thiol)

IT ***192126-76-4P***, Mycothiol
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); ***PUR (Purification or recovery)***; BIOL (Biological study); PREP (Preparation); PROC (Process)
(structure of U17 (mycothiol) isolated from Streptomyces clavuligerus and its properties as an antioxidant thiol)

RN 192126-76-4 ZCAPLUS

CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-mercapto-1-oxopropyl]amino]-2-deoxy-α-D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L95 ANSWER 11 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:34449 ZCAPLUS Full-text
DOCUMENT NUMBER: 108:34449
TITLE: Purification of thiols from biological samples
AUTHOR(S): Newton, Gerald L.; Fahey, Robert C.
CORPORATE SOURCE: Dep. Chem., Univ. California, San Diego, La Jolla, CA, 92093, USA
SOURCE: Methods in Enzymology (1987), 143(Sulfur Sulfur Amino Acids), 96-101
CODEN: MENZAU; ISSN: 0076-6879
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A 2-step purification procedure is described that allows a low-mol.-weight thiol component in a biol. extract to be isolated as the monobromobimane derivative in highly purified form. The thiols present in a deproteinized extract were first isolated on a thiol-agarose gel by a thiol-***disulfide*** exchange reaction. The thiols were then eluted with dithiothreitol and derivatized with monobromobimane. The derivative was purified to homogeneity by preparative HPLC. A procedure for electrolytic reduction of the bimane derivative was developed that allows regeneration of the thiol form of the purified product. Application of the method is illustrated for isolation of a major thiol component found in Halobacterium halobium, the structure of which was shown to correspond to γ-glutamylcysteine.

CC 9-15 (Biochemical Methods)
IT ***Thiols, preparation***
RL: ***PUR (Purification or recovery)***; PREP (Preparation)
(purification of, from biol. samples)

L95 ANSWER 12 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:77583 ZCAPLUS Full-text
DOCUMENT NUMBER: 64:77583
ORIGINAL REFERENCE NO.: 64:14585g-h
TITLE: Specificity of the dihydroxydinaphthyl disulfide (DDD) reaction
AUTHOR(S): Gabler, W.; Scheuner, G.
CORPORATE SOURCE: Karl Marx Univ., Leipzig, Germany
SOURCE: Acta Histocherm. (1966), 23(1-4), 102-9
DOCUMENT TYPE: Journal
LANGUAGE: German

AB The DDD reaction between protein-bound SH groups and the reagent 2,2'-dihydroxy-6,6'-dinaphthyl disulfide was said to be specific, except for some interference by 6-mercapto-2-naphthol produced during the reaction. High concns, of SH groups gave a blue, low concns, a red color reaction with Fast Blue B salt. Pretreatment of tissue slices with chloramine T greatly

intensified the color of the DDD reaction when different oxidizing agents were compared. Esterification of primary carboxyl groups produced an intense blue-violet color which might be mistaken for a high concentration of SH or SS groups. The reaction is not understood. 21 references.

CC 60 (Biochemical Methods)

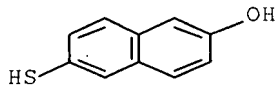
IT ***Mercapto group***
(in proteins, reaction with 2,2'-dihydroxy-6,6'-dinaphthyl disulfide)

IT ***6088-50-2***, 2-Naphthol, 6-mercapto-
(in protein bound mercapto group reaction with 2,2'-dihydroxy-6,6'-dinaphthyl disulfide)

IT ***6088-50-2***, 2-Naphthol, 6-mercapto-
(in protein bound mercapto group reaction with 2,2'-dihydroxy-6,6'-dinaphthyl disulfide)

RN 6088-50-2 ZCAPLUS

CN 2-Naphthalenol, 6-mercapto- (9CI) (CA INDEX NAME)



L95 ANSWER 13 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:50882 ZCAPLUS

DOCUMENT NUMBER: 52:50882

ORIGINAL REFERENCE NO.: 52:9214g-h

TITLE: ***Reduction*** of organic ***disulfides***

INVENTOR(S): Gutcho, Marcia; Laufer, Louis

PATENT ASSIGNEE(S): United States of America, as represented by the Secy. of the Navy

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2820780		19580121	US 1953-389479	19531030

AB Acid-insol. metallic sulfides of mol. weight over 60 (especially those of Bi, Pb, and Hg) catalyze the reaction of H2S with organic ***disulfides*** , RSSR' (R and R' may be amino acid, peptide, alkyl, or aryl groups), to produce their ***thiols***, RSH and R'SH. The reduction proceeds at room temperature and atmospheric pressure and the sulfide may be pre-formed or formed in situ. To 6% aqueous solution of oxidized glutathione (GSSG) 10 is added 10% aqueous solution Pb(OAc)2.3H2O 1 part and H2S is bubbled into the solution After the PbS is removed by filtration, GSH may be recovered as its Cu salt. Using H2S, cystine is reduced to cysteine in 75% yield. Similarly, with Bi2S3, 2,2'-dihydroxy-6,6'-dinaphthyl ***disulfide*** yields 70% 2,6-thionaphthol.

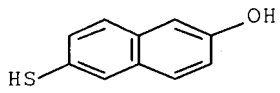
CC 10 (Organic Chemistry)

IT ***6088-50-2P***, 2-Naphthol, 6-mercapto-
RL: PREP (Preparation)
(preparation of)

IT ***6088-50-2P***, 2-Naphthol, 6-mercapto-
RL: PREP (Preparation)
(preparation of)

RN 6088-50-2 ZCAPLUS

CN 2-Naphthalenol, 6-mercapto- (9CI) (CA INDEX NAME)



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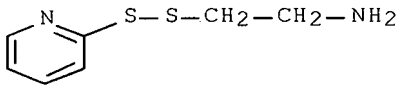
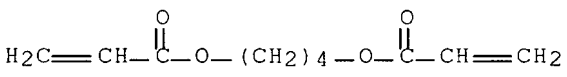
L95 ANSWER 14 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 145:460148 CASREACT Full-text
TITLE: Synthesis of Poly(β-amino ester)s with Thiol-Reactive Side Chains for DNA Delivery
AUTHOR(S): Zugates, Gregory T.; Anderson, Daniel G.; Little, Steven R.; Lawhorn, Ingrid E. B.; Langer, Robert
CORPORATE SOURCE: Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (2006), 128(39), 12726-12734
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The safe and efficient delivery of DNA remains the major barrier to the clin. application of non-viral gene therapy. Here, we present novel, biodegradable polymers for gene delivery that are capable of simple graft modification and demonstrate the ability to respond to intracellular conditions. We synthesized poly(β-amino ester)s using a new amine monomer, 2-(pyridyldithio)-ethylamine (PDA). These cationic, degradable polymers contain pyridyldithio functionalities in the side chains that react with high specificity toward thiol ligands. This reactivity is demonstrated using both mercaptoethylamine (MEA) and the thiol peptide RGDC, a ligand that binds with high affinity to certain integrin receptors. These two polymer derivs. displayed strong DNA binding as determined using electrophoresis and dye exclusion assays. In addition, the MEA-based polymer and plasmid DNA were shown to self-assemble into cationic complexes with effective diams. as low as 100 nm. Furthermore, this DNA binding ability was substantially reduced in response to intracellular glutathione concns., which may aid in DNA unpackaging inside the cell. These complexes also displayed low cellular toxicity and were able to mediate transfection at levels comparable to PEI in human hepatocellular carcinoma cells. These results suggest that PDA-based poly(β-amino ester)s may serve as a modular platform for polymer-mediated gene delivery.

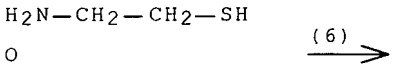
RX(6) OF 18 ...***F*** + I + ***O*** ===> ***P*** + ***Q***



F

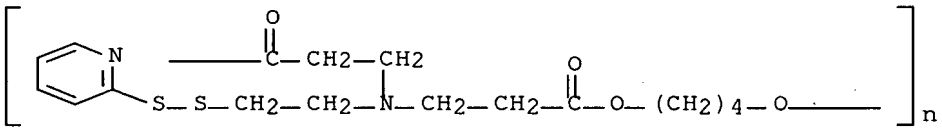


I

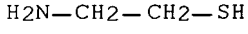


O

(6)



P
reaction produ
ct with mercap
toethylamine o



Q
reaction produ
ct with 2-(Pyr
idyldithio)-et

RX(6) RCT F ***83578-21-6,*** I 1070-70-8

STAGE(1)
CON 2 days, 60 deg C

STAGE(2)
RCT O ***60-23-1***
SOL 67-68-5 DMSO
CON room temperature

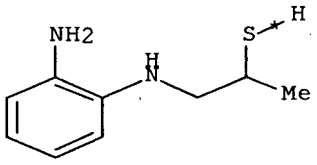
PRO P ***913399-31-2D,*** Q ***60-23-1D***
NTE no solvent (first stage)

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 15 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:378542 CASREACT Full-text
TITLE: Characterisation and biodistribution of two neutral 99mTc(CO)3 complexes with a tridentate ligand
AUTHOR(S): Rattat, Dirk; Cleynhens, Bernard; Bormans, Guy; Terwinghe, Christelle; Verbruggen, Alfons
CORPORATE SOURCE: Laboratory for Radiopharmaceutical Chemistry and Nuclear Medicine, Catholic University of Leuven, Louvain, 3000, Belg.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(19), 4192-4195
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB N-(2-Mercapto-propyl)-1,2-phenylenediamine (MPPDA) and N-β-aminoethylglycine (AEG) were labeled with 99mTc(CO)3+ to form the neutral complexes [99mTc(CO)3(MPPDA)] and [99mTc(CO)3(AEG)]. Both complexes were formed in excellent yields and their identities were confirmed by LC-MS. In mice, none of the new tracer agents showed brain uptake. [99mTc(CO)3(MPPDA)] was trapped mainly in the liver and excreted via the hepatobiliary system, whereas [99mTc(CO)3(AEG)] was excreted rapidly via the kidneys to the urine.

RX(2) OF 6 ...2 ***C*** + 2 ***D*** + ***E*** + 2 F ===>
G + ***H*** + ***I***



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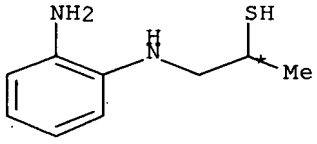

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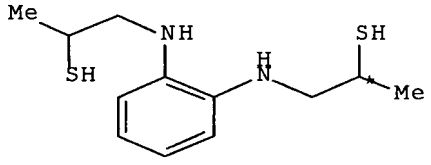

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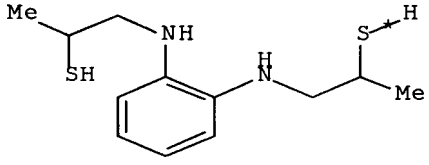

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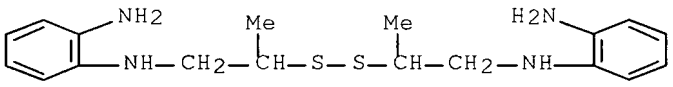

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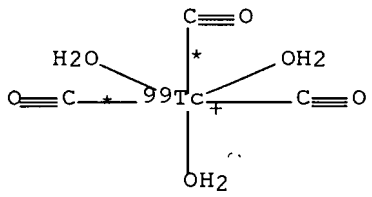
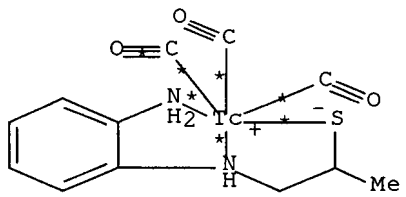
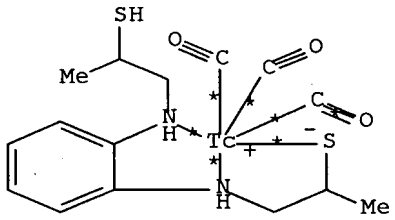


2 F

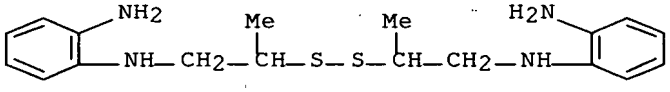
(2) ⟶



G
YIELD 57%



H
YIELD 27%



I
YIELD 17%
reaction product with technetium-99m triaq

RX(2) RCT C ***245059-12-5***, D ***255379-03-4***, E ***866395-63-3***, F 163932-31-8
PRO G 866395-64-4, H ***866395-65-5***, I 866395-63-3D
CON 30 minutes, 70 deg C, pH 10
NTE product with technetium-99m triaqua tricarbonyl

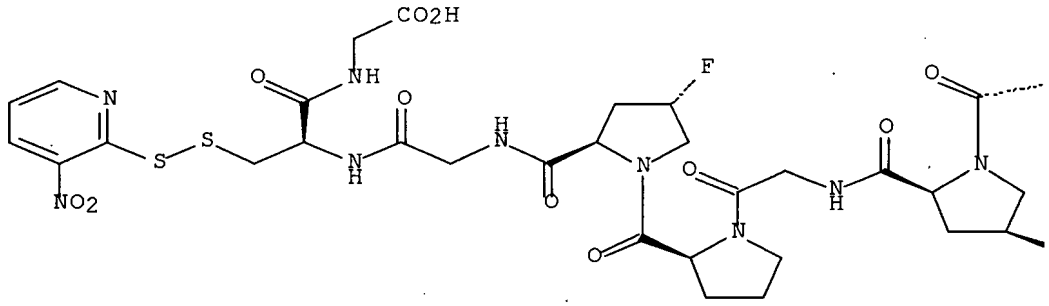
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 16 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 139:303501 CASREACT Full-text
TITLE: The role of cystine knots in collagen folding and stability, part I. Conformational properties of (Pro-Hyp-Gly)5 and (Pro-(4S)-FPro-Gly)5 model trimers with an artificial cystine knot
AUTHOR(S): Barth, Dirk; Musiol, Hans-Juergen; Schuett, Markus; Fiori, Stella; Milbradt, Alexander G.; Renner, Christian; Moroder, Luis
CORPORATE SOURCE: Max-Planck-Institut fuer Biochemie, Martinsried, 82152, Germany
SOURCE: Chemistry--A European Journal (2003), 9(15), 3692-3702
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In analogy to the cystine knots present in natural collagens, a simplified disulfide cross-link was used to analyze the conformational effects of a C-terminal artificial cystine knot on the folding of collagenous peptides consisting of solely (Pro-Hyp-Gly) repeating units. Assembly of the α chains into a heterotrimer by previously applied regioselective disulfide-bridging strategies failed because of the high tendency of (Pro-Hyp-Gly)5 peptides to self-associate and form homotrimers. Only when side-chain-protected peptides were used, for example in the Hyp(tBu) form, and a new protection scheme was adopted, selective interchain-disulfide crosslinking into the heterotrimer in organic solvents was successful. This unexpected strong effect of the conformational properties on the efficiency of well-established reactions was further supported by replacing the Hyp residues with (4S)-fluoroproline, which is known to destabilize triple-helical structures. With the related [Pro-(4S)-FPro-Gly]5 peptides, assembly of the heterotrimer in aqueous solution proceeded in a satisfactory manner. Both the intermediates and the final fluorinated heterotrimer are fully unfolded in aqueous solution even at 4°. Conversely, the disulfide-crossbridged (Pro-Hyp-Gly)5 heterotrimer forms a very stable triple helix. The observation that thermal unfolding leads to scrambling of the disulfide bridges was unexpected. Although NMR expts. support an extension of the triple helix into the cystine knot, thermolysis is not associated with the unfolding process. In fact, the unstructured fluorinated trimer undergoes an equally facile thermodegrdn. associated with the intrinsic tendency of unsym. disulfides to disproportionate into sym. disulfides under favorable conditions. The exptl. results obtained with the model peptides fully support the role of triple-helix nucleation and stabilization by the artificial cystine knot as previously suggested for the natural cystine knots in collagens.

RX(37) OF 170 COMPOSED OF RX(19), RX(20)
RX(37) ***AU*** + ***AY*** ===> ***BD***

PAGE 1-A



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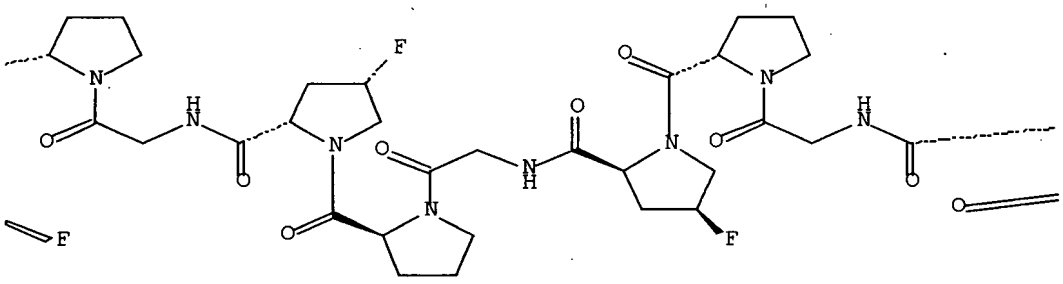

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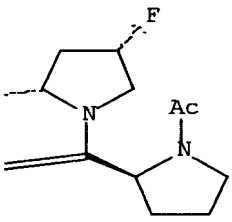

AU

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

2
STEPS
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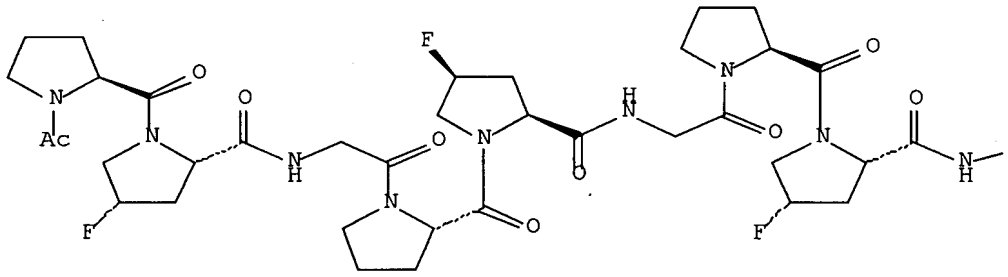
PAGE 1-A



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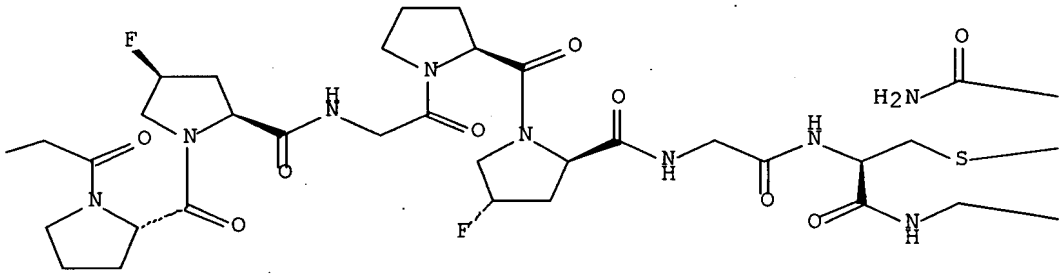

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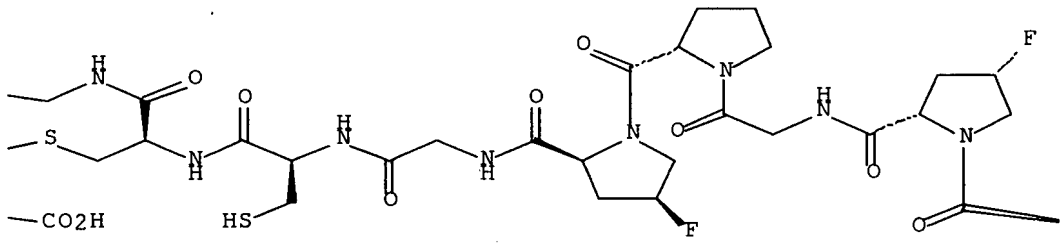

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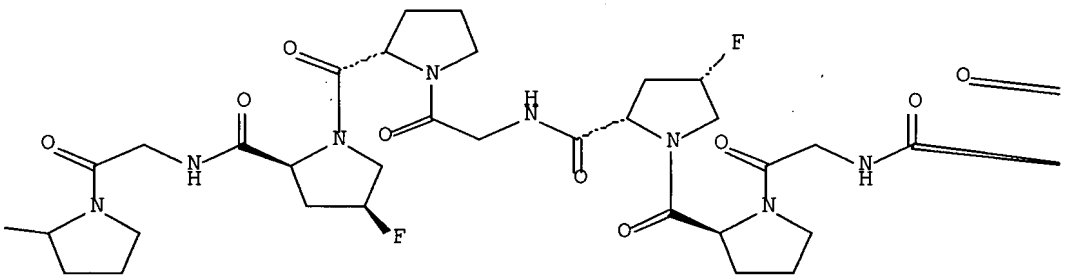

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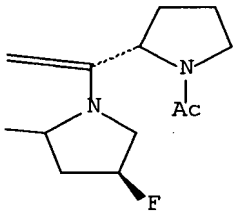


BD
YIELD 100%

RX(19) RCT AU ***610301-61-6***, AY ***610301-64-9***
PRO BC 610301-67-2
SOL 7732-18-5 Water
CON 6 hours, room temperature

RX(20) RCT BC 610301-67-2
RGT C 76-05-1 F3CCO2H, D 617-86-7 Et3SiH
PRO BD ***610301-68-3***
SOL 7732-18-5 Water
CON 5 minutes, room temperature
REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 17 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 139:180245 CASREACT Full-text
TITLE: Synthesis of novel acceptor substrates for the dolichyl phosphate mannose synthase from yeast
AUTHOR(S): Sprung, Ines; Carmes, Laurence; Watt, Gregory M.; Flitsch, Sabine L.
CORPORATE SOURCE: School of Chemistry Centre for Protein Technology, The University of Edinburgh, Edinburgh, EH9 3JJ, UK
SOURCE: ChemBioChem (2003), 4(4), 319-332
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dolichols are polyisoprenoid lipid components of mammalian membranes consisting of an average of 20 head-to-tail linked isoprene units of which the first isoprene is fully saturated The unusual size of these lipids is intriguing and poses questions about the role of dolichol structure in biol. processes. In order to probe structure and function we have synthesized potential dolichyl analogs that retain only the first two isoprene units and carry a second functional group within the terminal lipid chain. Such analogs were evaluated as substrates for a key enzyme in the dolichyl-dependent pathway of glycan biosynthesis, dolichyl phosphate mannose (Dol-P-Man) synthase. It was shown that some functional groups, including labels such as biotin, could be tolerated. When the synthetic analogs were attached to a solid support they were still substrates for the Dol-P-Man system and thus allowed the enzymic solid-phase synthesis of glycolipids.

RX(72) OF 517 COMPOSED OF RX(34), RX(33)
RX(72) ***CM*** + ***CA*** + 2 CE + ***CF*** ===>
CG + ***CH***

STRUCTURE DIAGRAM IS NOT AVAILABLE

CM: CM 2
reaction produ
cts with merca
ptopropionylam

RX(34) RCT CM ***68517-67-9D***

STAGE(1)
SOL 7732-18-5 Water
CON 15 minutes, room temperature

STAGE(2)
RCT CA 503844-00-6
SOL 64-17-5 EtOH, 7732-18-5 Water
CON 16 hours, room temperature

STAGE(3)
RGT BB 76-05-1 F3CCO2H
CON 10 minutes, room temperature

PRO CD 581778-62-3D
NTE solid-supported reaction, second stage is attachment to resin

RX(33) RCT CD 581778-62-3D, CE 3123-67-9

STAGE(1)
RGT CI 7786-30-3 MgCl2, CJ 1185-53-1 (HOCH2)3CNH2.HCl, CK 9002-93-1 Ortho-Gynol
CAT 62213-44-9 Mannosyltransferase, guanosine diphosphomannose-dolichol phosphate
SOL 7732-18-5 Water

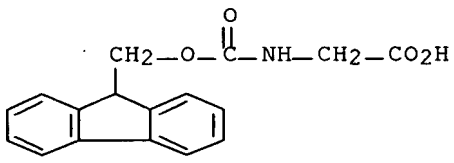
CON 21 hours, 37 deg C

STAGE(2)
RCT CF 60-24-2
SOL 7732-18-5 Water
CON 16 hours, 50 deg C

PRO CG ***581778-63-4***, CH ***503844-07-3***
NTE biotransformation, enzymic, buffered soln.
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 18 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 135:358149 CASREACT Full-text
TITLE: Improved Synthesis of C-Terminal Peptide Thioesters on "Safety-Catch" Resins Using LiBr/THF
AUTHOR(S): Quaderer, Richard; Hilvert, Donald
CORPORATE SOURCE: Laboratory of Organic Chemistry, Swiss Federal Institute of Technology (ETH), Zurich, CH-8092, Switz.
SOURCE: Organic Letters (2001), 3(20), 3181-3184
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The alkanesulfonamide "safety-catch" resin has proven useful for Fmoc-based synthesis of C-terminal peptide thioesters. We now report that the yield of isolated thioester can increase significantly when the cleavage reaction is carried out in 2M LiBr/THF rather than DMF or THF. The largest effects are seen with problematic peptides that aggregate or form secondary structures on the resin.

RX(2) OF 3 A + B + C + 2 D + E + F + ***G*** + 2 H + 2 ***N*** + AD ===> ***AE*** + ***AF***



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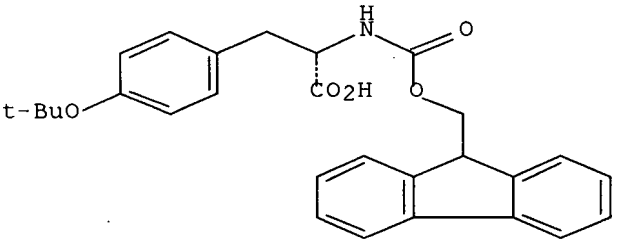

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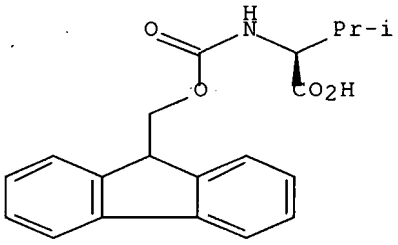

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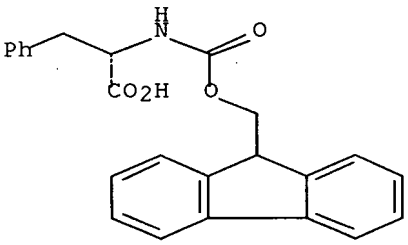

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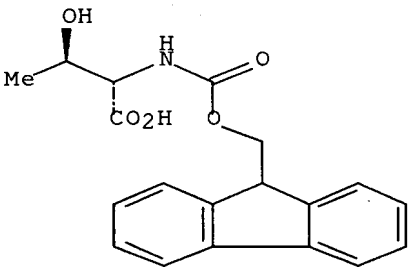

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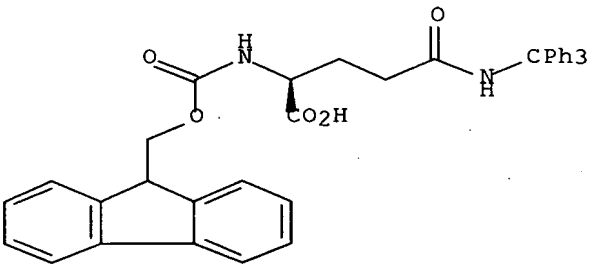

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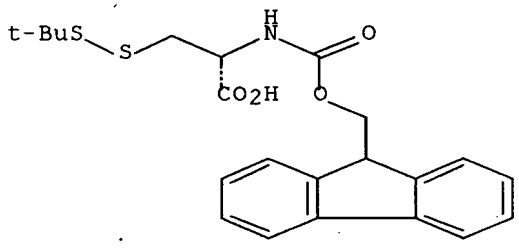
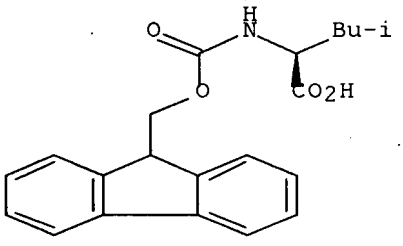
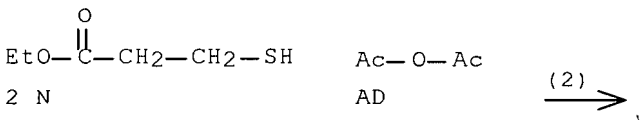


G



2 H



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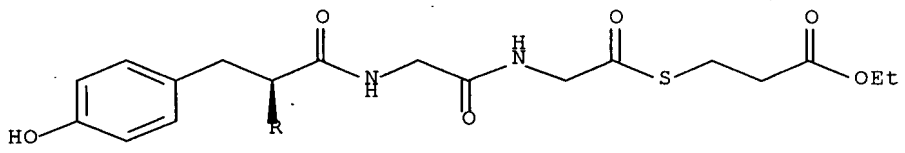

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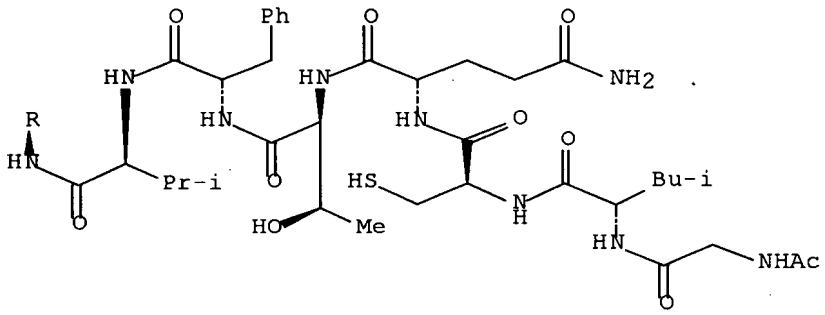


AE

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 1-B

—OEt

PAGE 2-A

AF

RX(2) RCT A 29022-11-5

STAGE(1)
RGT P 128625-52-5 Benzotriazolol P der, Q 7087-68-5 EtN(Pr-i)2
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(3)
RCT B 71989-38-3
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(4)
RCT C 68858-20-8
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(5)
RCT D 35661-40-6
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(6)
RCT E 73731-37-0
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q

7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(7)
RCT F 132327-80-1
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(8)
RCT G ***73724-43-3***
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(9)
RCT H 35661-60-0
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(10)
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(11)
RGT T 24424-99-5 (Boc)2O

STAGE(12)
RGT U 18107-18-1 Me3SiCH:N2
SOL 110-54-3 Hexane, 109-99-9 THF

STAGE(13)
RCT N ***5466-06-8***
RGT V 7550-35-8 LiBr
CAT 930-69-8 PhSNa
SOL 109-99-9 THF

STAGE(14)
RGT W 76-05-1 F3CCO2H, X 108-95-2 PhOH, Y 6485-79-6 Silane, tris(1-methylethyl)-
SOL 76-05-1 F3CCO2H, 7732-18-5 Water

STAGE(15)
RCT AD 108-24-7

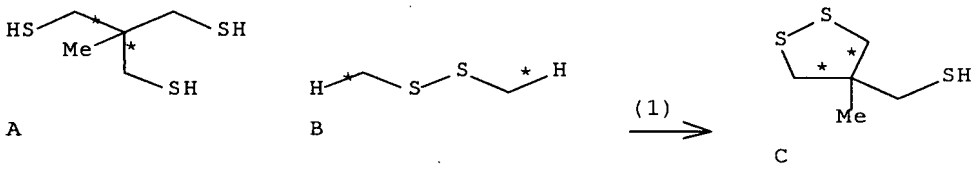
PRO AE ***372955-83-4***, AF ***372955-84-5***
NTE solid-supported reaction, first stage is attachment to 4-sulfamylbutyryl aminomethyl polystyrene (AM) resin, alternative cleavage conditions gave lower yield, peptide synthesis solvent assumed, 25% overall yield, piperidine deprotection after each addn.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 19 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 135:115927 CASREACT Full-text
TITLE: {2Fe3S} clusters related to the di-iron sub-site of

the H-centre of all-iron hydrogenases
AUTHOR(S): Razavet, Mathieu; Davies, Sian C.; Hughes, David L.; Pickett, Christopher J.
CORPORATE SOURCE: Department of Biological Chemistry, John Innes Centre, Norwich, NR4 7UH, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (9), 847-848
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The 1st synthetic {2Fe3S} clusters structurally related to the sub-site of the H-center of the all-iron hydrogenases, [Fe2(CO)5{(SCH2)2C(CH3)CH2SR}] (R = Me, CH2Ph),are prepared and characterized by x-ray crystallog. In the complexes tripodal dithiolate thioether ligands gave di-iron pentacarbonyls with differential (2:3) S-ligation of the Fe atoms.

RX(1) OF 20 ***A*** + ***B*** ===> ***C***...



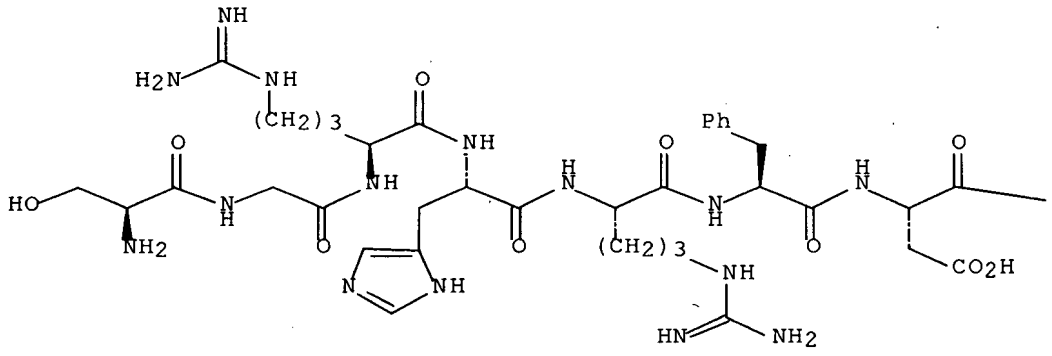
RX(1) RCT A ***39597-87-0***, B ***624-92-0***
PRO C ***110206-42-3***
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 20 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 134:237823 CASREACT Full-text
TITLE: Synthesis and conformational analysis of the insulin-like 4 gene product
AUTHOR(S): Bullesbach, Erika E.; Schwabe, C.
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, Medical University of South Carolina, Charleston, SC, 29425, USA
SOURCE: Journal of Peptide Research (2001), 57(1), 77-83
CODEN: JPERFA; ISSN: 1397-002X
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Insulin-like 4 (INSL-4) is a protein expressed in the early placenta. Its primary structure is insulin-like with reference to the distribution of cysteine residues and the single chain pro-form. Insulin-like 4 was generated by solid-phase peptide synthesis of the two chains followed by the sequential synthesis of the three disulfide bonds. Two disulfide isomers were produced, one with an insulin-like disulfide bonding pattern and the other with a reversed chain orientation. The CD spectra of the two disulfide isomers were

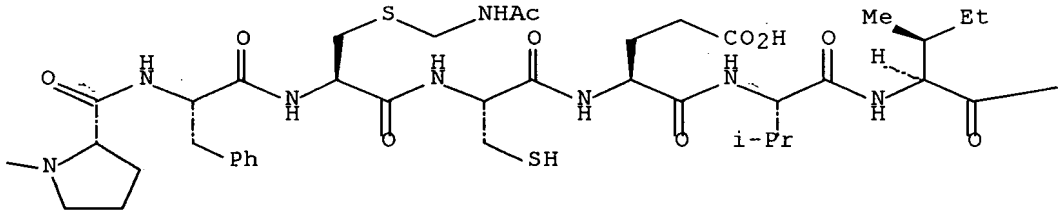
indistinguishable without any features produced by periodic structures. In addition, the hydrodynamic properties of the two isomers were identical which implied a very open structure of the disulfide-bonded two-chain mols. It appears that insulin-likeness cannot be defined solely on the basis of the primary structure of cDNA.

RX(3) OF 3 COMPOSED OF RX(1), RX(2)
RX(3) ***A*** + M ===> ***N***

PAGE 1-A



PAGE 1-B



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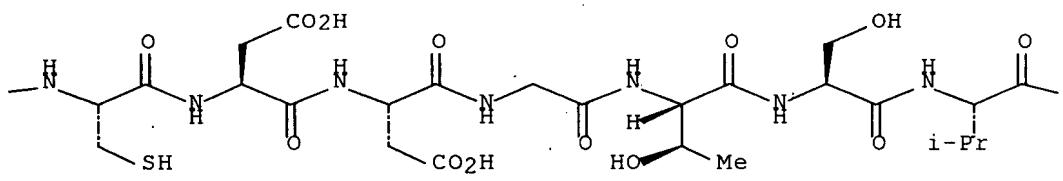

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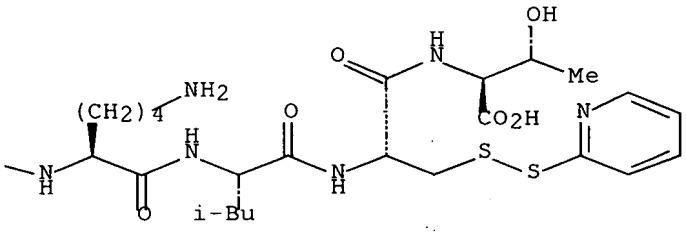


A

STRUCTURE DIAGRAM IS NOT AVAILABLE

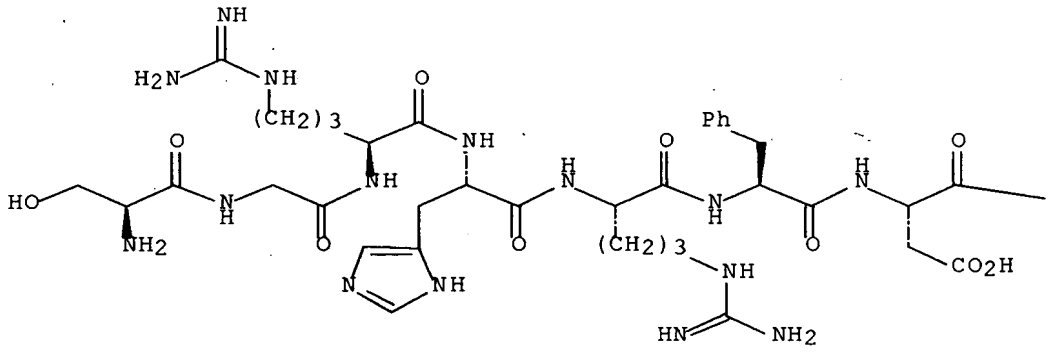
M

2 STEPS

STRUCTURE DIAGRAM IS NOT AVAILABLE

N: CM 1

PAGE 1-A



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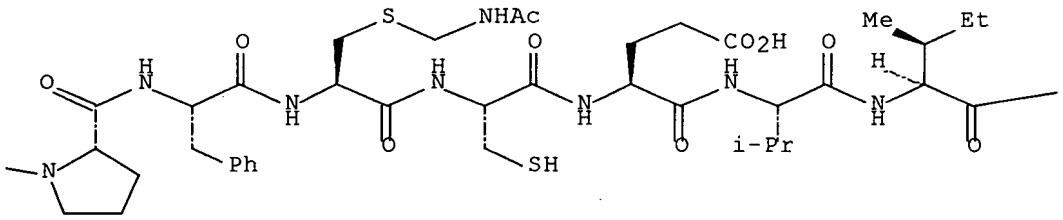

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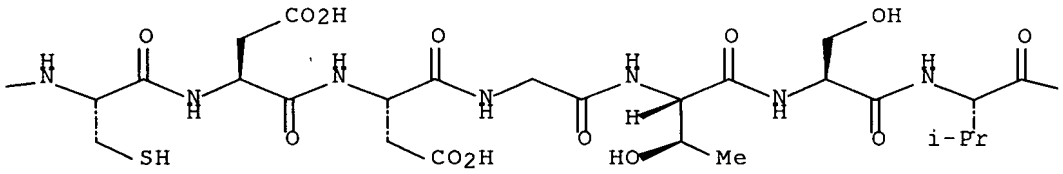
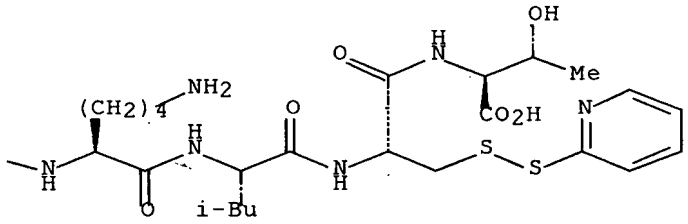


PAGE 1-D



N: CM 2

RX(1) RCT A ***330548-24-8***

STAGE(1)
SOL 64-19-7 AcOH

STAGE(2)
RGT C 7553-56-2 I2
SOL 64-19-7 AcOH

STAGE(3)
RGT D 50-81-7 (L)-Ascorbic acid
SOL 7732-18-5 Water

STAGE(4)
RGT E 2127-03-9 2-Pyridyl disulfide, F 100-68-5 PhSMe
SOL 76-05-1 F3CCO2H

STAGE(5)
RGT G 1493-13-6 F3CSO2H
SOL 76-05-1 F3CCO2H

STAGE(6)
RGT H 631-61-8 NH4OAc
SOL 75-05-8 MeCN

PRO B 209249-20-7
NTE stereoselective

RX(2) RCT B 209249-20-7, M 330625-42-8

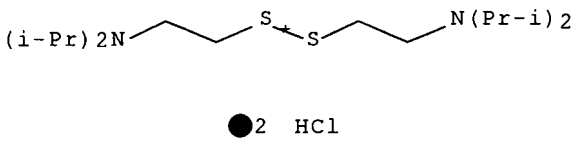
STAGE(1)
RGT O 1066-33-7 NH4 bicarbonate
SOL 7732-18-5 Water

STAGE(2)
RGT I 64-19-7 AcOH

PRO N ***330637-72-4***
NTE stereoselective
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

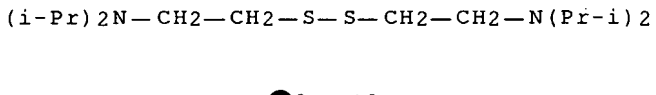
L95 ANSWER 21 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 132:49741 CASREACT Full-text
TITLE: Synthesis and mass spectral characterization of diisopropylamino-ethanethiol, -sulfides and -disulfides and vinyl sulfides
AUTHOR(S): Rohrbauch, D. K.; Berg, F. J.; Szafraniec, L. J.; Rossman, D. I.; Durst, H. D.; Munavalli, S.
CORPORATE SOURCE: Edgewood Research Development and Engineering Center, Aberdeen Proving Ground, U.S. Army, Aberdeen, MD, 21010, USA
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1999), 149, 95-106
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The sulfur containing chemical agent, O-ethyl-S-2-(diisopropylaminoethyl)methylph osphonothiolate, is an extremely potent inhibitor of the enzyme acetylcholinesterase and exhibits extended neurol. effects. It undergoes degradation on standing alone or in the environment. Hence, identification of its primary degradation products assumes considerable importance. The synthesis and mass spectral fragmentation behavior of the title compds., some of which are present in the O-ethyl-S-2-(diisopropylaminoethyl)methyl phosphonothiolate degradation products, has not received much attention. This communication describes the synthesis and mass spectral characterization of the title compds.

RX(2) OF 2 3 ***G*** + ***H*** ===> ***I*** + ***J*** + ***K***



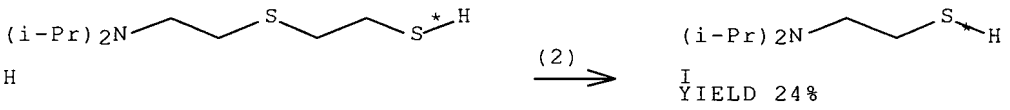
●2 HCl

2 G



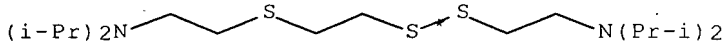
●2 HCl

G

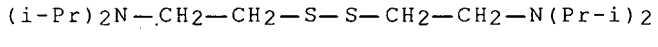


H

I
YIELD 24%



J
YIELD 27%



K
YIELD 31%

RX(2) RCT G ***252963-82-9***

STAGE(1)
RGT L 7791-25-5 SO2Cl2
SOL 75-09-2 CH2Cl2

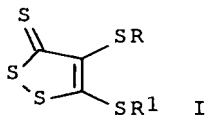
STAGE(2)
RCT H ***168885-96-9***
SOL 75-09-2 CH2Cl2

STAGE(3)
RGT M 1310-73-2 NaOH
SOL 7732-18-5 Water

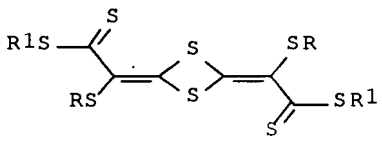
PRO I ***5842-07-9***, J ***110501-59-2***, K ***65332-44-7***

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 22 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 129:189320 CASREACT Full-text
TITLE: Synthesis and stereochemistry of bis(dithiacrown ether)- and dodecylthio-substituted (E)-thiodesaurines
AUTHOR(S): Rudershausen, Sandra; Drexler, Hans-Joachim; Holdt, Hans-Juergen
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Rostock, Rostock, D-18051, Germany
SOURCE: Journal fuer Praktische Chemie/Chemiker-Zeitung (1998), 340(5), 450-454
CODEN: JPCCEM; ISSN: 0941-1216
PUBLISHER: Johann Ambrosius Barth
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



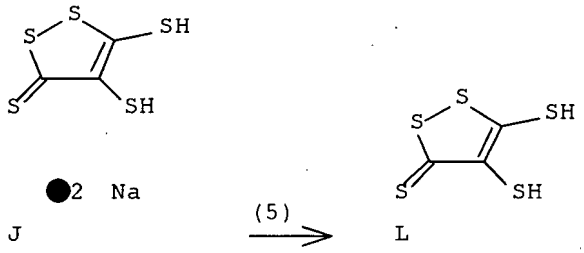
I



II

AB Reductive dimerization of 1,2-dithiole-3-thiones I [R = dodecyl, R1 = Me; R, R1 = dodecyl; RR1 = CH2(CH2OCH2)nCH2, n = 2-4] with P(OEt)3 furnished the corresponding thiodesaurines II. The stereochem. of II [RR1 = CH2(CH2OCH2)nCH2, n = 3] was determined by x-ray crystallog. anal.

RX(5) OF 17 ***J*** ===> ***L...***

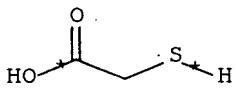


RX(5) RCT J ***100890-76-4***
RGT M 7647-01-0 HCl
PRO L ***69995-95-5***
SOL 7732-18-5 Water

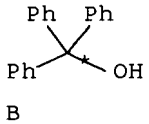
L95 ANSWER 23 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 125:47583 CASREACT Full-text
TITLE: N10-(2'-Mercaptoethanoyl)-2,2,5,5-tetramethyl-3,4-diathia-7,10-diazabicyclo[5.3.0]decane and its reaction with oxotrichlorobis(triphenylphosphine)rhenium(V)
AUTHOR(S): Alarabi, H.; Bell, R. A.; Howard-Lock, H. E.; Kowanetz, J.; Lock, C. J. L.
CORPORATE SOURCE: Lab. Inorganic Med., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
SOURCE: Canadian Journal of Chemistry (1996), 74(4), 574-582
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ligand mol. N10-(2'-mercaptoethanoyl)-2,2,5,5-tetramethyl-3,4-dithia-7,10-diazabicyclo[5.3.0]decane was prepared and characterized by 1H and 13C NMR spectroscopy and by mass spectrometry. The protected analog, N10-[(2'-triphenylmethylthio)ethanoyl]-2,2,5,5-tetramethyl-3,4-dithia-7,10-diazabicyclo[5.3.0]decane dimethanol hemihydrate, was examined by the same techniques and also by x-ray crystallog. Crystals were triclinic, P.hivin.1, a 11.125(2), b 11.986(2), c 13.562(3) Å, α 103.54(3), β 90.29(3), γ 107.11(3)°, and Z = 2. The crystal was unstable in air at room temperature, so measurements were made on a crystal sealed in a tube that contained MeOH vapor. The structure was solved by direct methods and refined to R = 0.1497, Rw = 0.0655 based on 5000 independent reflections. The high residuals were caused by solvent disorder. Bond lengths and angles were normal. The reaction of the ligand with ReOCl3(PPh3)2 yielded an unexpected asym. complex, oxo(1,1-dimethyl-1,8-dimercapto-3,6-diazaoctan-7-onato- N3,N6,S1,S8)rhenium. Crystals were monoclinic, space group P21/n, a 10.633(2), b 11.221(2), c 11.678(1) Å, β 116.10(1)°, Z = 4. The structure was solved by the heavy atom method and refined to R = 0.0471, Rw = 0.0340 based on 2866 unique reflections. Most bond lengths and angles were normal. The Re.tplbond.O distance of 1.681(5) Å was longer than normal. It is postulated that this was caused by competitive π bonding between the deprotonated amidic N atom and the Re atom, as shown by the short Re-N distance (1.997(6) Å) compared to the equivalent distance for the amine N atom (Re-N, 2.151(4) Å).

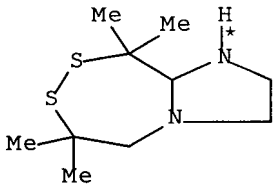
RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)
RX(6) **A** + B + **E** ===> **I**



A

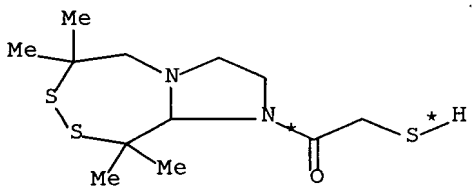


B



E

3 STEPS →



I
YIELD 75%

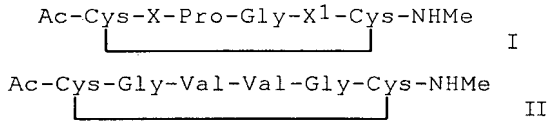
RX(1) RCT A ***68-11-1***, B 76-84-6
RGT D 64-19-7 AcOH
PRO C 34914-36-8
NTE 20-70.deg.

RX(2) RCT C 34914-36-8, E ***108168-04-3***
RGT G 538-75-0 DCC
PRO F 178113-10-5
SOL 75-09-2 CH2Cl2

RX(3) RCT F 178113-10-5
RGT J 76-05-1 F3CCO2H, K 617-86-7 Et3SiH
PRO I ***178113-13-8***
NTE 20.deg.

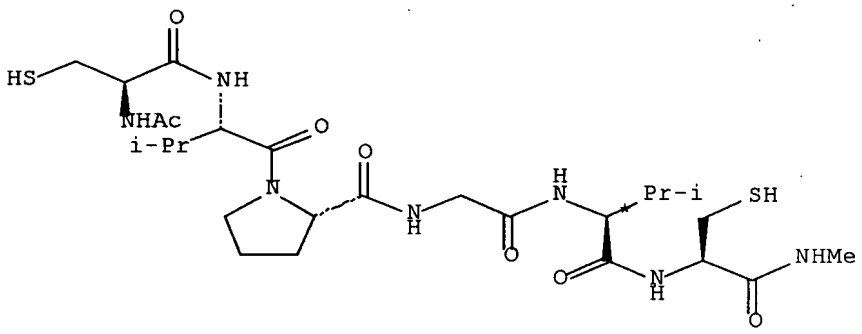
L95 ANSWER 24 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 109:190804 CASREACT Full-text
TITLE: Chain reversals in model peptides: studies of cystine-containing cyclic peptides. II. Effects of valyl residues and possible i-to-(i + 3) attractive ionic interactions on cyclization of [Cys1],[Cys6] hexapeptides
AUTHOR(S): Milburn, P. J.; Meinwald, Y. C.; Takahashi, S.; Oi, T.; Scheraga, H. A.
CORPORATE SOURCE: Baker Lab. Chem., Cornell Univ., Ithaca, NY, 14853-1301, USA
SOURCE: International Journal of Peptide & Protein Research

(1988), 31(3), 311-21
CODEN: IJPPC3; ISSN: 0367-8377
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



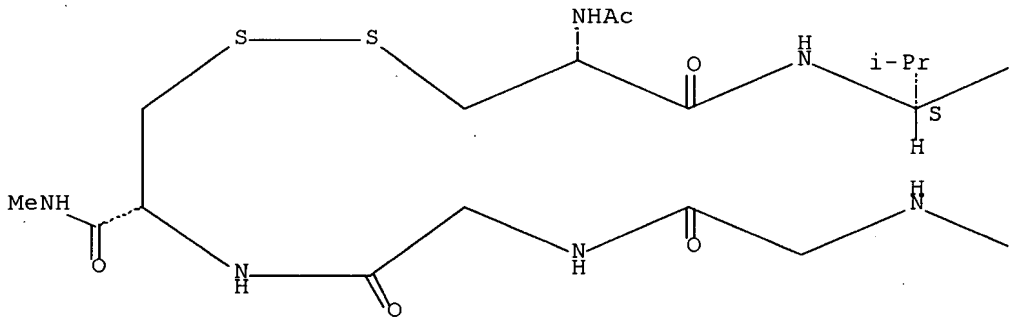
AB The synthesis of cystine-containing hexapeptides I (X = Glu, X1 = Lys; X = Lys, X1 = Glu; X = X1 = Val) and II is described. These were used in disulfide-exchange reactions with peptide I (X = Val, X1 = Gly) as the formal oxidant. The relative propensities for peptide cyclization were thus deduced, and the tendency toward the formation of chain-reversal conformations was established. quant. Ac-Cys-(Val)4-Lys-NHMe was prepared but was never obtained as the cyclic monomer, demonstrating that the formation of chain-reversals in this peptide was of very low probability. Incorporation of pairs of valyl residues decreased the ease of cyclization, but conformational flexibility in the cystine-containing hexapeptides may have compensated for substitutions which hinder the adoption of certain β-turn conformations. The peptides containing ionic residues were cyclized more readily than expected, and this process was relatively insensitive to salt concentration This observation is discussed with regard to the stabilization of β-turns by i to (i + 3) ionic interactions in peptides and proteins. A method for blocking thiols was introduced as an important in the anal. of the equilibrium mixts.

RX(35) OF 210 ***AY*** + ***BA*** ===> ***AR*** + ***BB***

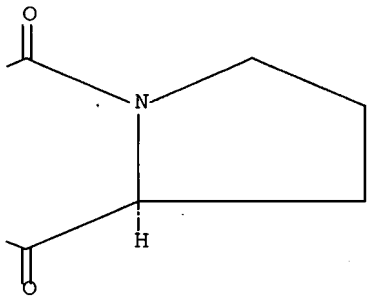


AY

PAGE 1-A



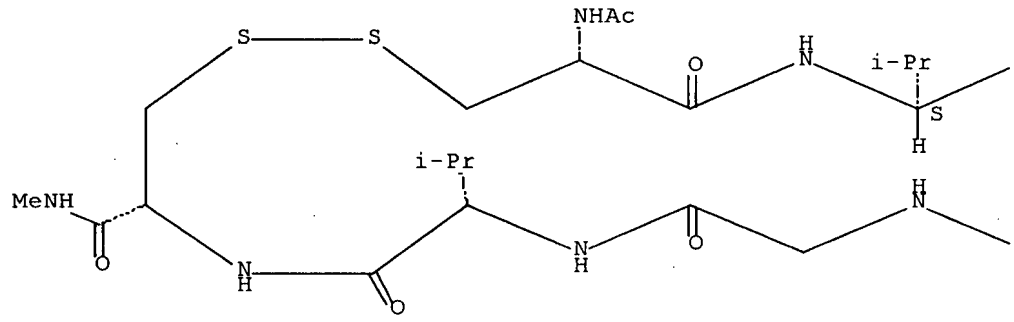
PAGE 1-B

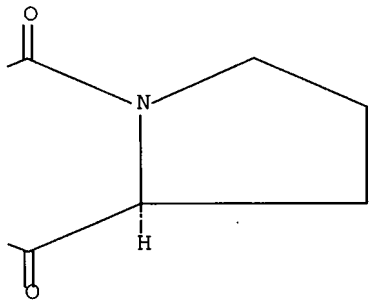


BA

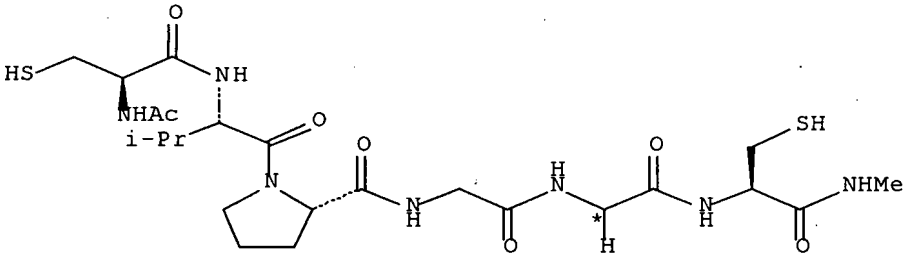
(35)

PAGE 1-A





AR



BB

RX(35) RCT AY ***117049-00-0***, BA ***108594-51-0***
PRO AR ***117048-95-0***, BB ***117049-02-2***
NTE equil., pH 8.0 buffer

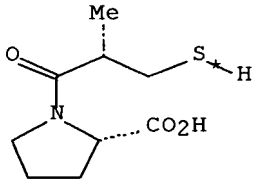
L95 ANSWER 25 OF 25 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 103:6696 CASREACT Full-text
TITLE: A nuclear magnetic resonance study of the formation and conformational equilibria of symmetrical and mixed disulfides of captopril
AUTHOR(S): Rabenstein, Dallas L.; Theriault, Yvon
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Canadian Journal of Chemistry (1985), 63(1), 33-9
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The oxidation of captopril (CpSH) [1-(D-3-mercapto-2-methylpropanoyl)-L-proline] by glutathione disulfide (GSSG) via thiol/disulfide exchange to form, in the first step, CpSSG and GSH and, in the second step, CpSSCp and GSH, has been studied in aqueous solution by 1H NMR. Due to slow rotation around the amide bond(s) of CpSH and CpSSCp and of the captopril part of CpSSG, sep. resonances are observed for the cis and trans conformations across these bonds. Conformational equilibrium consts. were estimated as a function of pH for CpSH, CpSSCp, and CpSSG from the intensities of resonances for the cis and

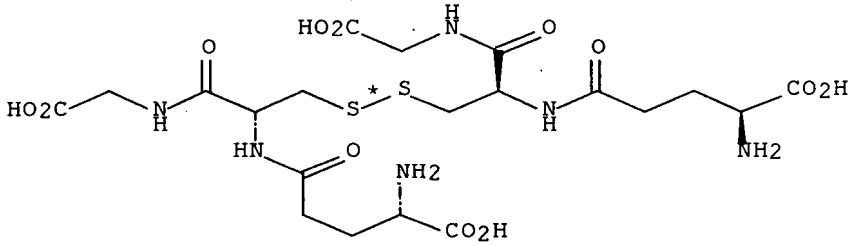
trans isomers. These equilibrium consts. were used in the determination of equilibrium consts. for the two steps in the oxidation of CpSH by GSSG. CpSH has a greater tendency to reduce disulfide bonds by thiol/disulfide exchange at physiol. pH, and thus form mixed disulfides, than do the thiol groups in amino acids. Also, the conformational equilibrium constant indicate that, at phys. pH, approx. two thirds of the captopril, either free or in a disulfide form has the trans conformation.

RX(1) OF 3 ***A*** + 2 ***B*** ===> ***C*** + ***D***

...

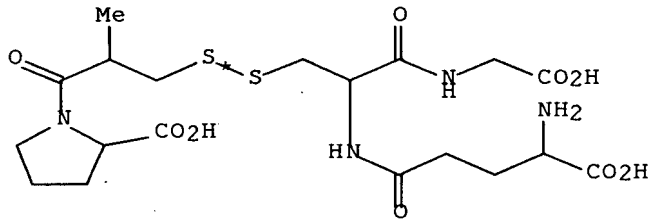


A

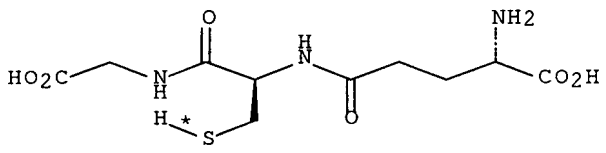


2 B

(1) →



C



D

RX(1) RCT A ***62571-86-2***, B ***27025-41-8***
RGT E 7447-40-7 KCl, F 75-65-0 t-BuOH, G 139-33-3 Di-Na EDTA
PRO C ***78636-30-3***, D ***70-18-8***
SOL 7789-20-0 D2O

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=> d his full

     (FILE 'HOME' ENTERED AT 13:46:45 ON 28 SEP 2007)

     FILE 'ZCAPLUS' ENTERED AT 13:46:57 ON 28 SEP 2007
                E US2007/APPS
                E US2007-569710/APPS
L*** DEL       1 S US2007-569710/AP
                D SCA
                E US2006-569710/APPS
                E WO2004-2774/APPS
                E WO2004-IB2774/APPS
L2             1 SEA ABB=ON  PLU=ON  WO2004-IB2774/AP
                SEL RN
                D IALL L2

     FILE 'REGISTRY' ENTERED AT 13:50:07 ON 28 SEP 2007
L3             1 SEA ABB=ON  PLU=ON  192126-76-4
                D SCA
L4             1 SEA ABB=ON  PLU=ON  3483-12-3
                D SCA
L5             1 SEA ABB=ON  PLU=ON  709044-44-0
                D SCA
L6             1 SEA ABB=ON  PLU=ON  847493-45-2
                D SCA
L7             1 SEA ABB=ON  PLU=ON  70-18-8
                D SCA
L8             1 SEA ABB=ON  PLU=ON  6088-50-2
                D SCA
L9             1 SEA ABB=ON  PLU=ON  105988-28-1
                D SCA
L10            1 SEA ABB=ON  PLU=ON  847493-44-1
                D SCA
L11            1 SEA ABB=ON  PLU=ON  847493-46-3
                D SCA

     FILE 'ZCAPLUS' ENTERED AT 13:57:44 ON 28 SEP 2007
L12            9 SEA ABB=ON  PLU=ON  L8 OR L10
                D SCA
                E THIOLS+ALL/CT
L13        26734 SEA ABB=ON  PLU=ON  THIOLS+OLD/CT
L14       264757 SEA ABB=ON  PLU=ON  PUR/RL
L15           32 SEA ABB=ON  PLU=ON  L13 (L) L14
                E DISULFIDES+ALL/CT
L16       118162 SEA ABB=ON  PLU=ON  DISULFID?/BI
L17          147 SEA ABB=ON  PLU=ON  DI SULFID?/BI
L18         1626 SEA ABB=ON  PLU=ON  BISULFID?/BI OR BI SULFID?/BI
L19           11 SEA ABB=ON  PLU=ON  L15 AND (L16 OR L17 OR L18)
                D SCA
                E DISULFIDES+ALL/CT
L20         3625 SEA ABB=ON  PLU=ON  DISULFIDES/CT
L21            7 SEA ABB=ON  PLU=ON  L20 (L) L14
L22       167140 SEA ABB=ON  PLU=ON  ?THIOL?/BI
L23            1 SEA ABB=ON  PLU=ON  L21 AND L22
                D SCA
L24       120255 SEA ABB=ON  PLU=ON  ?DISULFID?/BI
L25       167140 SEA ABB=ON  PLU=ON  ?THIOL?/BI
L26        20268 SEA ABB=ON  PLU=ON  L24 AND L25
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L27      856378 SEA ABB=ON  PLU=ON  ?PURIF?/BI
L28        1351 SEA ABB=ON  PLU=ON  L26 AND L27
L29       97550 SEA ABB=ON  PLU=ON  ?GLUTATHION?/BI
L30         253 SEA ABB=ON  PLU=ON  L28 AND L29
L31          14 SEA ABB=ON  PLU=ON  (L3 OR L5 OR L6 OR (L8 OR L9 OR L10 OR
                L11)) AND L26
                D SCA
L32           4 SEA ABB=ON  PLU=ON  L19 AND 75-15-0?/OBI
                D SCA
L33           7 SEA ABB=ON  PLU=ON  L19 NOT L32
                D SCA
L34           7 SEA ABB=ON  PLU=ON  L21 NOT L33
                D SCA
                D SCA L21
                E MERCAPTANS+ALL/CT
                D SCA L31
L35           2 SEA ABB=ON  PLU=ON  L31 AND ?ISOLAT?/OBI
L36           1 SEA ABB=ON  PLU=ON  L31 AND TOTAL/TI
L37           1 SEA ABB=ON  PLU=ON  L31 AND REDUCTION?/TI
L38          10 SEA ABB=ON  PLU=ON  L33 OR L35 OR L36 OR L37
                D SCA
                D COST
L39      166847 SEA ABB=ON  PLU=ON  ?MERCAPT?/BI
L40       99071 SEA ABB=ON  PLU=ON  ?THIOL?/AB
L41       97340 SEA ABB=ON  PLU=ON  ?MERCAPT?/AB
L42       68341 SEA ABB=ON  PLU=ON  ?DISULFID?/AB
L43      618440 SEA ABB=ON  PLU=ON  ?PURIF?/AB
L44     1062429 SEA ABB=ON  PLU=ON  ?ISOLAT?/AB
L45        2544 SEA ABB=ON  PLU=ON  (L41 OR L40) AND  L42 AND (L43 OR L44)
L46         195 SEA ABB=ON  PLU=ON  L14 AND L45
                D KWIC 1
                D KWIC 50
L47          65 SEA ABB=ON  PLU=ON  L3
L48           1 SEA ABB=ON  PLU=ON  L46 AND L47
                D SCA
L49           1 SEA ABB=ON  PLU=ON  L8 AND L46
L50           1 SEA ABB=ON  PLU=ON  L9 AND L46
L51          19 SEA ABB=ON  PLU=ON  (L8 OR L9 OR L10)
L52          10 SEA ABB=ON  PLU=ON  L33 OR (L35 OR L36 OR L37)
L53          16 SEA ABB=ON  PLU=ON  L51 NOT L52
                D SCA
                E STEENCAMP D/AU
                E STEINCAMP D/AU
                D AU L2
                E STEENKAMP D/AU
L54          60 SEA ABB=ON  PLU=ON  STEENKAMP D?/AU
L55           2 SEA ABB=ON  PLU=ON  L52 AND L54
                D SCA
L56           3 SEA ABB=ON  PLU=ON  L28 AND L54
L57           1 SEA ABB=ON  PLU=ON  L56 NOT L55
                D SCA
                D SCA L23
L58           3 SEA ABB=ON  PLU=ON  L39 AND L21
                D SCA
L59           2 SEA ABB=ON  PLU=ON  L5
L60           1 SEA ABB=ON  PLU=ON  L6
L61           1 SEA ABB=ON  PLU=ON  L11
L62           2 SEA ABB=ON  PLU=ON  (L59 OR L60 OR L61)
                D SCA
L63           9 SEA ABB=ON  PLU=ON  L8
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L64           1 SEA ABB=ON  PLU=ON  L10
L65           9 SEA ABB=ON  PLU=ON  (L63 OR L64)
                D SCA
L66           6 SEA ABB=ON  PLU=ON  L65 AND MERCAPTO?/OBI
L67           6 SEA ABB=ON  PLU=ON  L65 AND MERCAPTO/OBI
L68       15061 SEA ABB=ON  PLU=ON  MERCAPTO GROUP/CT
L69           1 SEA ABB=ON  PLU=ON  L65 AND L68
L70           2 SEA ABB=ON  PLU=ON  L3 AND L45
                D SCA
L71           2 SEA ABB=ON  PLU=ON  L3/PUR
                D SCA
L72         993 SEA ABB=ON  PLU=ON  L20 (L) (RGT OR RCT OR RACT)/RL
L73        1831 SEA ABB=ON  PLU=ON  L13 (L) (PRU OR PREP)/RL
L74          32 SEA ABB=ON  PLU=ON  L13 (L) (PUR)/RL
L75          46 SEA ABB=ON  PLU=ON  L72 AND (L73 OR L74)
L76           1 SEA ABB=ON  PLU=ON  L74 AND L72
                D SCA
L77           0 SEA ABB=ON  PLU=ON  L21 AND L73
L78           0 SEA ABB=ON  PLU=ON  L21 AND L74
L79        1355 SEA ABB=ON  PLU=ON  L13 AND L20
L80          56 SEA ABB=ON  PLU=ON  L79 AND L45
L81      424326 SEA ABB=ON  PLU=ON  PURIF?/OBI
L82      287765 SEA ABB=ON  PLU=ON  ISOLAT?/OBI
L83           2 SEA ABB=ON  PLU=ON  L80 AND L81
L84           1 SEA ABB=ON  PLU=ON  L80 AND L82
L85           3 SEA ABB=ON  PLU=ON  (L83 OR L84)
                D SCA

     FILE 'CASREACT' ENTERED AT 16:32:54 ON 28 SEP 2007
                E A/FG.RCT
                E THI/FG.RCT
                E DISU/FG.PRO
L86        1384 SEA ABB=ON  PLU=ON  THIOL/FG.RCT (L) DISULFIDE/FG.PRO
                E DISULFIDE/FG.RCT
L87         505 SEA ABB=ON  PLU=ON  DISULFIDE/FG.RCT (L) THIOL/FG.PRO
L88         123 SEA ABB=ON  PLU=ON  L86 AND L87
L89          12 SEA ABB=ON  PLU=ON  L86 (L) L87
                D SCA

     FILE 'CAPLUS' ENTERED AT 16:38:03 ON 28 SEP 2007
L90          12 SEA ABB=ON  PLU=ON  L89
                D SCA
L91         123 SEA ABB=ON  PLU=ON  L88
L92          11 SEA ABB=ON  PLU=ON  (L43 OR L44) AND L91
                D SCA

     FILE 'REGISTRY' ENTERED AT 16:40:52 ON 28 SEP 2007

     FILE 'ZCAPLUS' ENTERED AT 16:40:57 ON 28 SEP 2007
                D STAT QUE L55
                D STAT QUE L56
L93           3 SEA ABB=ON  PLU=ON  L55 OR L56
                D IBIB ABS HITIND HITSTR L93 1-3

     FILE 'REGISTRY' ENTERED AT 16:41:51 ON 28 SEP 2007

     FILE 'ZCAPLUS' ENTERED AT 16:41:54 ON 28 SEP 2007
                D STAT QUE L33
                D STAT QUE L35
                D STAT QUE L36
```

```
                D STAT QUE L37
                D STAT QUE L23
                D STAT QUE L58
                D STAT QUE L62
                D STAT QUE L69
                D STAT QUE L71
L94           13 SEA ABB=ON  PLU=ON  (L33 OR L35 OR L36 OR L37 OR L23 OR L58 OR
                  L62 OR L69 OR L71) NOT (L55 OR L56)

     FILE 'CASREACT' ENTERED AT 16:43:08 ON 28 SEP 2007
                D STAT QUE L89

     FILE 'ZCAPLUS, CASREACT' ENTERED AT 16:43:37 ON 28 SEP 2007
L95           25 DUP REM L94 L89 (0 DUPLICATES REMOVED)
                     ANSWERS '1-13' FROM FILE ZCAPLUS
                     ANSWERS '14-25' FROM FILE CASREACT
                D IBIB ABS HITIND HITSTR L95 1-13
                D IBIB ABS FHIT L95 14-25

     FILE 'ZCAPLUS' ENTERED AT 16:46:11 ON 28 SEP 2007

     FILE 'ZCAPLUS, CASREACT' ENTERED AT 16:46:16 ON 28 SEP 2007
                D IBIB ABS FHIT L95 14-25


     FILE HOME

     FILE ZCAPLUS

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     FILE LAST UPDATED: 27 Sep 2007  (20070927/ED)

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       substance identification.

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     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   27 SEP 2007  HIGHEST RN 948530-59-4
     DICTIONARY FILE UPDATES:  27 SEP 2007  HIGHEST RN 948530-59-4

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FILE CAPLUS

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